

REC'D 29 MAY 2000

WIPO

27/9300/00384

PA 240106

# THE UNITED STATES OF AMERICA

TO ALL TO WHOM THESE PRESENTS SHALL COME:

UNITED STATES DEPARTMENT OF COMMERCE

United States Patent and Trademark Office 09/914451

May 04, 2000

THIS IS TO CERTIFY THAT ANNEXED HERETO IS A TRUE COPY FROM THE RECORDS OF THE UNITED STATES PATENT AND TRADEMARK OFFICE OF THOSE PAPERS OF THE BELOW IDENTIFIED PATENT APPLICATION THAT MET THE REQUIREMENTS TO BE GRANTED A FILING DATE UNDER 35 USC 111.

APPLICATION NUMBER: 60/122,110

FILING DATE: February 26, 1999

## PRIORITY DOCUMENT

SUBMITTED OR TRANSMITTED IN  
COMPLIANCE WITH RULE 17.1(a) OR (b)



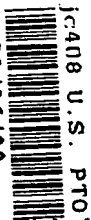
By Authority of the  
COMMISSIONER OF PATENTS AND TRADEMARKS

P. SWAIN  
Certifying Officer

PART ( / ) OF ( / ) PART(S)



02/26/99



Jc408 U.S. PTO

**PROVISIONAL APPLICATION COVER SHEET**Jc541 U.S. PTO  
60/122110

This is a request for filing a PROVISIONAL APPLICATION under 37 CFR 1.53(c).

|  |  |                  |       |   |  |                           |       |
|--|--|------------------|-------|---|--|---------------------------|-------|
| DOCKET NO.   |  | 54660-54661      |       | TYPE A PLUS SIGN (+)<br>INSIDE THIS BOX → |  | +                         |       |
| INVENTOR(S)/APPLICANT(S)   |  |                  |       |   |  |                           |       |
| LAST NAME  |  | FIRST NAME       |       | MIDDLE INITIAL                            | RESIDENCE<br>(CITY AND STATE OR FOREIGN COUNTRY) |                           |       |
| HAEGGSTROM   |  | Jesper           |       | Z.  | Stockholm, Sweden                                |                           |       |
| THUNNISSEN   |  | Marjolein        |       |   | Akersberga, Sweden                               |                           |       |
| NORDLUND   |  | Par              |       |   | Stockholm, Sweden                                |                           |       |
| TITLE OF THE INVENTION (280 characters max)                      |  |                  |       |   |  |                           |       |
| DRUG DESIGN BASED ON THE STRUCTURE OF LTA <sub>4</sub> HYDROLASE |  |                  |       |   |  |                           |       |
| CORRESPONDENCE ADDRESS   |  |                  |       |   |  |                           |       |
| YOUNG & THOMPSON<br>745 South 23rd Street<br>Arlington           |  |                  |       |   |  |                           |       |
| STATE  | VA   | ZIP CODE         | 22202 | COUNTRY                                   | USA  |                           |       |
| ENCLOSED APPLICATIONS PARTS (check all that apply)               |  |                  |       |   |  |                           |       |
| X  | Specifica-<br>tion   | No. of Pages     | 336   |   | Small Entity Statement                           |                           |       |
| X  | Drawing(s)   | No. of<br>Sheets | 14    | X   | Other (specify): 38 Claims and Abstract          |                           |       |
| METHOD OF PAYMENT (check one)                                    |  |                  |       |   |  |                           |       |
| X  | A check in the amount of \$150 to cover<br>the filing fee is enclosed.                               |                  |       | Check No.                                 |  | PROVISIONAL<br>FILING FEE | \$150 |
| X  | The Commissioner is hereby authorized to<br>charge the filing fee and credit Deposit<br>Account No.: |                  |       | 25-0120                                   |  |                           |       |

[ ] Additional inventors are being named on separately numbered sheets attached hereto.

The invention was made by an agency of the United States Government or under a contract with an agency of the United States Government.

[X] No.

[ ] Yes, the name of the U.S. Government agency and the Government contract number are:

Respectfully submitted,

Benoit Castel  
Reg. No. 35,041

February 26, 1999

**PROVISIONAL APPLICATION FILING ONLY**

Form Y&amp;T (1/98)



# DRUG DESIGN BASED ON THE STRUCTURE OF LTA<sub>4</sub> HYDROLASE

## 1. BACKGROUND

### 1.1 Technical field

The present invention relates to methods of design or identification of biologically active compounds, which methods are based on the first definition ever of a three-dimensional structure of a protein involved in the leukotriene cascade. Further, the invention relates to novel compounds obtained by said methods, to advantageous uses of such compounds as well as to processes for the preparation thereof.

### 1.2 Prior art

Leukotriene A<sub>4</sub> (LTA<sub>4</sub>) hydrolase is a pivotal enzyme in the biosynthesis of leukotrienes, a family of paracrine hormones implicated in the pathophysiology of inflammatory and allergic disorders, in particular bronchial asthma (Samuelsson, B. *Science* 220, 568-75 (1983); and Lewis, R.A., Austen, K.F. & Soberman, R.J. *N Engl J Med* 323, 645-55 (1990)). Leukotrienes are formed by immunocompetent cells including neutrophils, eosinophils, basophils, mast cells, and macrophages, in response to a variety of immunological as well as non-immunological stimuli. These lipid mediators are divided into two major classes exemplified by the chemotaxin LTB<sub>4</sub>, and the spasmogenic cysteinyl-leukotrienes (LTC<sub>4</sub>, LTD<sub>4</sub>, and LTE<sub>4</sub>). Leukotriene biosynthesis is initiated by the enzyme 5-lipoxygenase which converts arachidonic acid into the unstable epoxide LTA<sub>4</sub>, a central intermediate in the leukotriene cascade. LTA<sub>4</sub> may in turn be hydrolyzed into LTB<sub>4</sub> by the enzyme LTA<sub>4</sub> hydrolase, or conjugated with GSH to form LTC<sub>4</sub>, a reaction catalyzed by a specific LTC<sub>4</sub> synthase. During cellular activation, all key enzymes in leukotriene biosynthesis, except LTA<sub>4</sub> hydrolase, form a biosynthetic complex assembled at the nuclear membrane, suggesting that leukotrienes may have unknown intranuclear functions related to gene regulation or cell growth (Serhan, C.N., Haeggstrom, J.Z. & Leslie, C.C. *Faseb J* 10, 1147-58 (1996)).



Leukotriene B<sub>4</sub>, the natural product of LTA<sub>4</sub> hydrolase, is one of the most powerful chemotactic agents known to date and triggers leukocyte adherence and aggregation at only nM concentrations (Ford-Hutchinson, A.W., Bray, M.A., Doig, M.V., Shipley, M.E. & Smith, M.J.H. *Nature* **286**, 264-265 (1980)). Hence, this molecule is regarded as a key mediator of inflammation, and has been implicated in a number of diseases, including arthritis, psoriasis, inflammatory bowel disease (IBD), and chronic obstructive pulmonary disease (COPD). Furthermore, the role of LTB<sub>4</sub> in inflammation has been well corroborated by the anti-inflammatory properties of LTA<sub>4</sub> hydrolase inhibitors, particularly in combination with a cyclooxygenase inhibitor, and specific LTB<sub>4</sub> receptor antagonists, as well as the reduced inflammatory reactions observed in several animal models of leukotriene deficiency (Tsuji, F., Miyake, Y., Enomoto, H., Horiuchi, M., Mita, S. *Eur. J. Pharmacol.* **346**, 81-85, (1998); Chen, X.S., Sheller, J.R., Johnson, E.N. & Funk, C.D. *Nature* **372**, 179-182 (1994); Griffiths, R.J., *et al.* *Proc Natl Acad Sci U S A* **92**, 517-21 (1995); and Griffiths, R.J., *et al.* *J Exp Med* **185**, 1123-9 (1997)). In addition, LTB<sub>4</sub> modulates the immune response, *e.g.*, by interference with specific subsets of lymphocytes, production of cytokines, as well as liberation of immunoglobulins from B-lymphocytes (Payan, D.G., Missirlian-Bastian, A. & Goetzl, E.J. *Proc Natl Acad Sci U S A* **81**, 3501-5 (1984); Rola-Pleszczynski, M. & Lemaire, I. *J Immunol* **135**, 3958-61 (1985); and Yamaoka, K.A., Claesson, H.E. & Rosen, A. *J Immunol* **143**, 1996-2000 (1989)). Recent data also indicate that LTB<sub>4</sub> stimulates, and thus has a crucial role in the regulation of, cell proliferation and cell survival in HL-60 cells, suggesting that LTA<sub>4</sub> hydrolase inhibitors may have an anti-proliferative effect. (Dittman, K.H., Mayer, C., Rodemann, H.P., Petrides, P.E., and Denzlinger, C. *Leuk. Res.* **22**, 49-53 (1998)). The cell surface receptor for LTB<sub>4</sub> (BLTR) was recently cloned and found to be abundantly expressed in the immune system, including lymphocytes, spleen and thymus (Yokomizo, T., Izumi, T., Chang, K., Takuwa, Y. & Shimizu, T. *Nature* **387**, 620-624 (1997)). BLTR belongs to a family of chemokine receptors and, interestingly, together with CD4 it was found to be an efficient coreceptor for HIV-1 infection (Owman, C., *et al.* *Proc Natl Acad Sci U S*



A 95, 9530-4 (1998)). Moreover, LTB<sub>4</sub> is also a natural ligand to the nuclear orphan receptor PPAR $\alpha$ , suggesting that LTB<sub>4</sub> may have intranuclear functions possibly related to lipid homeostasis (Devchand, P.R., *et al. Nature* 384, 39-43 (1996)).

LTA<sub>4</sub> hydrolase is a cytosolic 69 kDa enzyme without any similarity to other soluble or membrane bound xenobiotic epoxide hydrolases (Funk, C.D., *et al. Proc Natl Acad Sci U S A* 84, 6677-81 (1987)). The enzyme's epoxide hydrolase activity, which generates LTB<sub>4</sub>, is highly substrate selective accepting only LTA<sub>4</sub> and to a small extent the double bond isomers LTA<sub>3</sub> and LTA<sub>5</sub>. Typically, LTA<sub>4</sub> hydrolase undergoes suicide inactivation and covalent modification when exposed to LTA<sub>4</sub> (Evans, J.F., Nathaniel, D.J., Zamboni, R.J. & Ford-Hutchinson, A.W. *J. Biol. Chem.* 260, 10966-10970 (1985)). During this process, LTA<sub>4</sub> apparently binds to Tyr-378, a residue which also seems to play a role for the formation of the critical *cis-trans-trans* geometry in the conjugated triene structure of LTB<sub>4</sub> (Mueller, M.J., *et al. Proc Natl Acad Sci U S A* 93, 5931-5935 (1996); and Mueller, M., Andberg, M., Samuelsson, B. & Haeggstrom, J. Z. *J. Biol. Chem.* 271, 24345-24348 (1996)).

From sequence comparisons with certain metalloproteases and aminopeptidases, a zinc binding motif (HEXXH-X<sub>18</sub>-E) was unexpectedly found in LTA<sub>4</sub> hydrolase (Vallee, B.L. & Auld, D.S. *Proc. Natl. Acad. Sci. USA* 87, 220-224 (1990)). Further studies demonstrated that the enzyme indeed contains one catalytic zinc atom complexed to His295, His299, and Glu318 (Medina, J.F., *et al. Proc. Natl. Acad. Sci. USA* 88, 7620-7624 (1991)). In addition, a previously unknown peptide cleaving activity was discovered which requires the presence of anions, particularly chloride (Haeggström, J.Z., Wetterholm, A., Medina, J.F. & Samuelsson, B. *J Lipid Mediator* 6, 1-13 (1993)). Although the endogenous physiological peptidase substrate(s) has not yet been identified, LTA<sub>4</sub> hydrolase cleaves certain arginyl di- and tripeptides with very high efficiency (Örning, L., Gierse, J.K. & Fitzpatrick, F.A. *J. Biol. Chem.* 269, 11269-11273 (1994)). Hence, LTA<sub>4</sub> hydrolase can be described as a



bifunctional zinc metalloenzyme with the unique ability to accept both lipid and peptide substrates. Using site-directed mutagenesis, Glu296 and Tyr383 were found to be critical for the peptidase reaction, presumably as a general base and proton donor, respectively (Blomster, M., Wetterholm, A., Mueller, M.J. & Haeggström, J.Z. *Eur. J. Biochem.* **231**, 528-534 (1995); and Wetterholm, A., *et al. Proc Natl Acad Sci U S A* **89**, 9141-9145 (1992)). Since the enzyme's ability to convert LTA<sub>4</sub> into LTB<sub>4</sub> was not affected by the mutations, the two enzyme activities of LTA<sub>4</sub> hydrolase are exerted via non-identical but overlapping active sites. Notably, unlike other enzymes in the leukotriene cascade, LTA<sub>4</sub> hydrolase is ubiquitous in mammalian cells and tissues suggesting that it may have other functions presumably related to its peptide cleaving activity.

As a consequence of the identification of LTA<sub>4</sub> hydrolase as a zinc metalloenzyme with a peptidase activity, it was observed that LTA<sub>4</sub> hydrolase is inhibited by bestatin, a general aminopeptidase inhibitor, and captopril, an inhibitor of angiotensin converting enzyme (Örning, L., *et al. J. Biol. Chem.* **266**, 16507-16511 (1991)).

Tsuge *et al.*, (*J. Mol. Biol.* **238**, 854-856 (1994)), have described the crystallization of LTA<sub>4</sub> hydrolase. However, despite the well recognized need thereof, the three-dimensional structure of LTA<sub>4</sub> hydrolase has not yet been disclosed. More specifically, the problems that need to be overcome in order to provide such a determination may in brief be explained as follows. There are two major difficulties in obtaining a three-dimensional structure of a protein molecule. The first one is to grow crystals of good quality that are reproducible and diffract to atomic resolution (beyond 2.5Å). This means a thorough and cumbersome investigation of parameters that influence the crystal growth such as pH, temperature, nature of buffers, nature of precipitant, just to mention a few. The addition of ligands such as substrate analogues or inhibitors or the addition of other molecules can be important for obtaining good crystals. There is only little understanding of the physical



background of the crystallisation process which means that the search for suitable crystallisation conditions for a certain protein is unique, requires creativity and intuition, and is governed by trial and error procedures. The purity of the protein is also a crucial parameter in the crystallisation and a suitable degree of purity can be hard, or even impossible, to achieve. The second major difficulty is associated with overcoming the phase-problem which is inherent to X-ray diffraction methods. To be able to overcome this problem it is necessary to substitute the protein with suitable heavy atom substance such as e.g. mercury, gold or platinum compounds. Crystals often cannot withstand the treatment with these compounds and the search for suitable substitutions is not straight forward and may become very exhaustive. Another option is to substitute all methionines by seleno-methionine (Se-Met) residues. This method requires production of recombinant protein in special strains of *E. coli* under non-standard conditions, followed by a new purification and recrystallisation of the Se-Met containing protein. Although Tsuge et al reported the crystallisation of LTA<sub>4</sub> hydrolase, their crystals only diffracted to medium resolution and the phase-problem was not solved. Thus, as a reliable definition of the three-dimensional structure of LTA<sub>4</sub> hydrolase would enable e.g. a display in visual form on a computer screen of the shape of the molecule, then, could the above mentioned problems be solved, a whole range of possibilities would be opened, such as rational structure-based drug design, e.g. in combination with combinatorial chemistry, aimed at production of novel medicaments useful in disorders associated with the leukotriene cascade, as well as protein-engineering to create novel variants of the enzyme with altered, but yet useful, catalytic properties.

As LTA<sub>4</sub> hydrolase is a recognized important drug target, some inhibitors thereof have been synthesized (Wetterholm, A., *et al. J Pharmacol Exp Ther* **275**, 31-7 (1995); and Yuan, W., Wong, C., Haeggstrom, J. Z., Wetterholm, A. & Samuelsson, B. *J. Am. Chem. Soc.*, **114**, 6552-6553 (1992)). Interestingly, certain inhibitors of LTA<sub>4</sub> hydrolase were reported to act also as LTB<sub>4</sub> receptor antagonists (Labaudinière R, Hilboll G, Leon-Lomeli A, Terlain B, Cavy F, Parnham M, Kuhl P, and Dereu N. *J. Med. Chem.* **35**, 3170-3179 (1992)). Due to the absence of any



available information regarding the three-dimensional structure of LTA<sub>4</sub> hydrolase, as discussed above, none of the previously described inhibitors have been designed based on the exact structure thereof. Accordingly, there is a need within this field of determining the three-dimensional structure of LTA<sub>4</sub> hydrolase in order to design more potent and selective inhibitors of LTA<sub>4</sub> hydrolase as well as modified structures exhibiting even more advantageous pharmaceutical properties.

## 2. THE PRESENT INVENTION

As the following chapter includes a substantial amount of text, it has herein been divided into separate sections, each one of which disclose separate aspects of the present invention.

### Index Chapter 2

#### 2.1 Summary of the invention

#### 2.2 Brief description of the drawings

#### 2.3 Definitions

#### 2.4 Detailed description of the invention

##### 2.4.1 LTA<sub>4</sub> hydrolase, subsequences and analogues thereof

##### 2.4.2 Compounds complementary to LTA<sub>4</sub> hydrolase

##### 2.4.3 A complex of LTA<sub>4</sub> hydrolase and a complementary compound

##### 2.4.4 Advantageous uses of LTA<sub>4</sub> hydrolase, complementary compounds and complexes thereof

##### 2.4.5 Screening for LTA<sub>4</sub> hydrolase analogues

###### 2.4.5 (a) Method

###### 2.4.5 (b) Analogues obtainable by the present screening method

###### 2.4.5 c) Mutated forms of LTA<sub>4</sub> hydrolase obtainable by the present screening method

###### 2.4.5 (d) Nucleic acids encoding the novel compounds

##### 2.4.6 (a) Production and purification of genetically modified forms of LTA<sub>4</sub> hydrolase

##### 2.4.6 (b) Purified LTA<sub>4</sub> hydrolase



## 2.4.7 Screening for LTA<sub>4</sub> hydrolase binding compounds

### 2.4.7 (a) Method

### 2.4.7 (b) Identified binding compounds

## 2.4.8 Protein engineering

### 2.4.8 (a) Method

### 2.4.8 (b) Novel specifically designed proteins

### 2.4.8 (c) Use of genetically modified LTA<sub>4</sub> hydrolase

## 2.4.1 Pharmaceutical applications of the present invention

### 2.4.9 (a) First medical indication

### 2.4.9 (b) Second medical indication and pharmaceutical methods

### 2.4.10 (c) Methods of treatment

## 2.5 A general production of the novel molecules

## 2.6 Detailed description of the drawings

### 2.1 Summary of the invention

The object of the present invention is to fulfill the above defined need. This has been achieved by the crystallization and determination of the three-dimensional structure of LTA<sub>4</sub> hydrolase complexed with the competitive inhibitor bestatin and subsequent structure determination of complexes between LTA<sub>4</sub> hydrolase and two specific inhibitors. It is the first three-dimensional structure of any protein component of the leukotriene cascade and enables a description of the structural basis and molecular mechanisms of various enzyme functions, such as the two catalytic activities of LTA<sub>4</sub> hydrolase. In addition, the structural information will now make possible rational design of enzyme inhibitors, which may be developed into clinically useful anti-inflammatory drugs.

### 2.2 Brief description of the drawings

Figure 1 shows the key enzymes and intermediates in leukotriene biosynthesis.

Figure 2 shows 2Fo-Fc density contoured at 1.1 σ. Part of the active site in the neighborhood of the bestatin molecules is shown.



Figure 3 is a ribbon diagram of the tertiary structure of leukotriene A<sub>4</sub> hydrolase.

Figure 4 (a) is a ribbon diagram of the N-terminal domain.

Figure 5 (a) is a ribbon diagram of the catalytic domain.

Figure 6 shows the structure of the C-terminal domain.

Figure 7 illustrates zinc binding ligands in LTA<sub>4</sub> hydrolase.

Figure 8 (a) is a Ball-and-Stick presentation of the binding of bestatin in LTA<sub>4</sub> hydrolase.

Figure 8 (b) is a schematic overview of bestatin binding in LTA<sub>4</sub> hydrolase.

Figure 9 (a) is a wire representation of the central cavity found in LTA<sub>4</sub> hydrolase (shown as C $\alpha$ -trace).

Figure 9 (b) is a schematic presentation for the proposed binding of LTA<sub>4</sub> into the cavity.

Figure 10 is a schematic representation for the proposed reaction mechanism of the epoxide hydrolase.

### 2.3 Definitions

In the present context, the term "the three-dimensional form adopted thereof in nature" is to be understood as the conformational structure, defined by the parameters x, y and z in a conventional coordinate system, that a naturally occurring molecule adapt under conditions where it is capable of exerting its biological activities. The specific conditions during which the herein presented data were collected are detailed in the section "Experimental".

The term "isolated" and variations thereof when used in connection with a molecule, such as protein, a polypeptide or a nucleic acid, means that said molecule is isolated from other substances, such as other proteins, DNA etc normally accompanying it in its natural environment.

The term "leukotriene A<sub>4</sub> (LTA<sub>4</sub>) hydrolase" as used herein is to be understood to include any mammalian or other LTA<sub>4</sub> hydrolase which comprises the same backbone as the human form specifically disclosed in the present application, irrespective of source. The amino acid sequences of mammalian LTA<sub>4</sub> hydrolase



have been shown to be identical to about 90%. Thus, the three-dimensional structures thereof may be suspected to be identical to approximately the same extent. "Thiolamine" and "hydroxamic acid" are used herein to denote the compounds exemplified in the Experimental section of the present specification.

A "complementary compound" means any compound, the structure of which enables a binding thereof to a specified protein, i.e a compound having a conformation or structure enabling such a suitable fit as to provide an energetically favorable interaction between protein-complementary compound.

"Analogue" means, as used herein, a chemically altered molecule which shares the backbone with, or at least structurally resembles, a "parent molecule". In the present specification, such a "parent molecule" may be LTA<sub>4</sub> hydrolase or an inhibitor thereof.

In the present application, the term "active site" is to be understood to include any region capable of binding a substrate and converting it into product.

The term "nucleic acid" refers to a deoxyribonucleotide or ribonucleotide polymer in either single- or double-stranded form, and unless otherwise limited, encompasses known analogs of nucleotides, that can function in a similar manner as naturally occurring nucleotides.

The phrase "hybridising specifically to" refers to the binding, duplexing, or hybridising of a molecule only to a particular nucleotide sequence under stringent conditions when that sequence is present in a complex mixture (*e.g.*, total cellular) of DNA or RNA. The term "stringent conditions" refers to conditions under which a probe will hybridise to its target subsequence, but to no other sequences. Stringent conditions are sequence-dependent and will be different in different circumstances. Longer sequences hybridise specifically at higher temperatures. Generally, stringent conditions are selected to be about 5°C lower than the thermal melting point  $T_m$  for the specific sequence at a defined ionic strength and pH. The  $T_m$  is the temperature (under defined ionic strength, pH, and nucleic acid concentration) at which 50% of the probes complementary to the target sequence hybridise to the target sequence at equilibrium. (As the target sequences are generally present in excess, at  $T_m$ , 50% of the probes are occupied at equilibrium). Typically, stringent conditions will be those



in which the salt concentration is less than about 1.0 M Na ion, typically about 0.01 to 1.0 M Na ion concentration (or other salts) at pH 7.0 to 8.3 and the temperature is at least about 30°C for short probes (*e.g.*, 10 to 50 nucleotides) and at least about 60°C for long probes (*e.g.*, greater than 50 nucleotides). Stringent conditions may also be achieved with the addition of destabilizing agents such as formamide. "Essentially pure" means herein a purity of at least about 80%, especially at least about 90% and preferably at least about 95%, such as 98-99%. The purity of LTA<sub>4</sub> hydrolase, an analogue or inhibitor thereof is according to the present invention preferably determined by general biochemical and biophysical methods well-known to the skilled in this field. For proteins, SDS polyacrylamide gel electrophoresis (SDS-PAGE) with Coomassie and silver staining or amino acid sequence analysis can be used, whereas high-pressure liquid chromatography (HPLC), gas chromatography coupled to mass spectrometry (GC-MS), and nuclear magnetic resonance spectroscopy (NMR) are suitable methods for small organic molecules (peptides, lipids, or carbohydrates, or combinations of these classes of substances).

## 2.4 Detailed description of the invention

### 2.4.1 LTA<sub>4</sub> hydrolase, subsequences and analogues thereof

In a first aspect, the present invention relates to an isolated protein comprising at least a subsequence of the amino acid sequence of leukotriene A<sub>4</sub> (LTA<sub>4</sub>) hydrolase, which subsequence has the corresponding three-dimensional form adopted thereof in nature. The protein according to invention as discussed below and elsewhere in this application is also understood to encompass any other functionally equivalent part, derivative or conformational analogue thereof. More specifically, the invention relates to the above disclosed protein which comprises a subsequence of the amino acid sequence of leukotriene A<sub>4</sub> (LTA<sub>4</sub>) hydrolase, which is able to participate in, and influence, *e.g.* by providing enzymatic activity, the leukotriene cascade. Most preferably, the protein according to the invention is capable of controlling said cascade by exerting an enzymatic activity and thus regulate the production of leukotriene B<sub>4</sub> (LTB<sub>4</sub>). In a particular embodiment, the protein is comprised of essentially all of the amino acid sequence of leukotriene A<sub>4</sub> (LTA<sub>4</sub>) hydrolase as



disclosed in SEQ ID NO 1, or a functionally equivalent part, derivative or conformational analogue thereof.

Thus, the present invention relates to an isolated LTA<sub>4</sub> hydrolase in its naturally occurring three-dimensional form. More specifically, the present application provides a listing illustrating, for the first time, the coordinates defining human LTA<sub>4</sub> hydrolase complexed to an inhibitor thereof. Thus, the coordinates defining the conformation of LTA<sub>4</sub> hydrolase have been determined by the present inventors as complexed with bestatin, thiolamine and hydroxamic acid, respectively. Bestatin is a universal inhibitor of amino peptidase activity, while the last mentioned two are specific inhibitors of LTA<sub>4</sub> hydrolase. Based on these different activities, said inhibitors may be used as models in the design of novel molecules having desired properties. Methods for such design will be discussed in further detail below as a further advantageous aspect of the invention. For reasons of convenience for the reader of the present specification, the data collection comprising the novel coordinates according to the invention is included in the present description as a separate section denoted "X-ray data", as Tables 9-11, immediately preceding the claims. In said tables, atom no 1 to atom no 4876 define the LTA<sub>4</sub> hydrolase part of the complex. In table 9, atom no 4882 to atom no 5463 relate to bestatin. (Bestatin has been thoroughly discussed in the literature, see e.g. Mathé, G. *Biochem. Pharmacol.* 45, 49-54 (1991).) The intervening atoms relate to the metals that bind in LTA<sub>4</sub> hydrolase, i.e. the active site Zn atom and the Yb atoms that were crucial for the present structure determination. The conditions prevailing at the determination thereof will be described in detail in the Experimental section below. As the skilled in this field realises, such coordinates usually exhibit a certain degree of variation, due to e.g. thermal motion and slight differences in crystal packing. Thus, any references herein to Tables 9-11 in connection with the proteins and other molecules are merely intended to illustrate the coordinates defining the conformation of the molecules under identical conditions, as determined by use of the same apparatus and method. Accordingly, this embodiment of the invention is not limited to a molecule having exactly the specified coordinates, but rather to



molecules capable of adopting such a structure. For example, a human LTA<sub>4</sub> hydrolase according to the invention will exhibit a strong bit a conformational similarity with the coordinates presented by atom nos 1 - 4876 of Tables 9-11, wherein a variation of about 1%, or 0.5 Å, may be expected. Accordingly, any such variants are within the scope of the present invention.

As regards amino acid sequence, in a specific embodiment, the protein according to the invention is identical, by direct sequence comparison, to at least about 50%, more specifically, at least about 70%, such as at least about 90%, to the LTA<sub>4</sub> hydrolase as defined by SEQ ID NO. 1 while in the three-dimensional form adopted thereof in nature. In this context, it is noted that the amino acid sequence of LTA<sub>4</sub> hydrolase also appears from the data of Tables 9-11, but is also included as a separate sequence listing for reasons of clarity. The protein of this embodiment of the invention are e.g. variants originating from any species, preferably mammals, such as humans, mice or other rodents, etc. Alternatively, the variants including subsequences of the human sequence are mutated forms, resulting from either spontaneous mutations or deliberately produced mutations, as discussed in more detail below.

One preferred embodiment of the present invention is a protein which comprises at least one of the regions defined below in Tables 1-3 below as active sites.

Table 1: Residues lining the big cavity from outside to insite

|   | Left wall      | Right wall                                |
|---|----------------|---|
| 1 |                | Lys608, Asp606, Lys605,<br>Lys354, Thr355 |
| 2 | Phe356, Phe362 | Gln544, Asp573, Lys572, Arg568            |
| 3 | Val376         | Lys565, Arg540, Leu507                    |



|   |   |   |
|---|---|---|
| 4 | Ser380, Ser352, Glu348                    | Pro569                                    |
| 5 | Tyr378, Glu348                            | Arg563, Glu533, Phe536,<br>Arg537, Tyr267 |
| 6 | Tyr383, Phe314, Glu318, Glu384,<br>Arg326 |   |
| 7 | Gly268, Gly269, Met270                    | His295, Asn341, Phe340                    |
| 8 | Ser288, His497                            | Glu325, Asn291                            |

In Table 1, Lys565, Ser380, Pro569, Glu533, Tyr383, Phe314, Glu318, Glu384, Arg326, Gly268, Gly269, Met270, His295, Phe340, Ser288, and Glu325 are strictly conserved amino acids, while Lys608, Phe356, Phe362, Lys572, Arg568, Tyr378, Phe536, Tyr 267, and Asn291 are conserved in nature.

Table 2: Amino-acids in the bestatin binding site ("basic" amino-peptidase site)

The binding of bestatin to LTA<sub>4</sub> hydrolase is described by way of coordinates in Table 9. Below follows the specific amino acids involved in the binding of bestatin and similar structures.

Gln136

Ala137

Tyr267

Gly268

Gly269

Met270

Glu271

Val292

His295

Glu296

His299

Glu318



Tyr378  
Tyr383  
Arg563  
Lys565

Table 3: Amino acids in the leukotriene binding site

The present amino acids define the site binding leukotriene-based inhibitors, such as thiolamine and hydroxamic acid, as shown in Tables 10 and 11, respectively.

Gln136  
Ala137  
Tyr267  
Gly268  
Gly269  
Met270  
Glu271  
Val292  
His295  
Glu296  
His299  
Trp315  
Glu318  
Val322  
Phe362  
Val367  
Leu369  
Pro374  
Asp375  
Ile372  
Ala377  
Pro382



Tyr378

Tyr383

Arg563

Lys565

In Tables 1-3 above, the enumeration of the amino acid sequence of LTA<sub>4</sub> hydrolase begin without the initial Met. Thus, compared to SEQ ID NO 1, which includes the initial Met, the amino acid enumeration above is lowered by one. Accordingly, Gln136 above corresponds to Gln 137 of SEQ ID NO 1, Ala137 above corresponds to Ala 138 of SEQ ID NO 1, etc.

Table 4: General catalytic domain for the M1 class of enzymes

Amino acids no. 210-450.

The present region will provide a basis for the development of enzyme inhibitors useful in the control other biological pathways than the leukotriene cascade.

Thus, as regards the above defined region of aminopeptidase activity of LTA<sub>4</sub> hydrolase, the present inventors have surprisingly observed, that said region is in fact universal for all enzymes belonging to the metallohydrolase family denoted M1. Thus, this specific subsequence of LTA<sub>4</sub> hydrolase is encompassed by the present invention as a novel protein *per se*. In addition to the various advantageous uses of subsequences of LTA<sub>4</sub> hydrolase described herein in connection with the leukotriene cascade, this region, which is shared between all M1 enzymes, will find several further applications in connection with other enzymatic pathways. For example, the present region, herein denoted the "M1 region" in order to clarify that it is shared between the M1 enzymes, may advantageously be used to produce synthetic inhibitors, or identify natural inhibitors, of any one of the other M1 enzymes. Such M1 inhibitors will be discussed below when compounds complementary to LTA<sub>4</sub> hydrolase are disclosed.



The above disclosed proteins and peptides comprising subunits of LTA<sub>4</sub> hydrolase are advantageously used e.g. as enzymes or more preferably in methods wherein novel inhibitors of enzymatic activities are identified and/or designed.

#### 2.4.2 Compounds complementary to LTA<sub>4</sub> hydrolase

In a second aspect, the present invention relates to a novel compound defined by a structure substantially complementary to the above described protein, preferably identified by use of the novel LTA<sub>4</sub> hydrolase conformation according to the present invention. The complementary compound is a naturally occurring or synthetic protein, peptide, lipid, carbohydrate or any other organic or inorganic compound. In relation to naturally occurring compounds, it is to be understood that the present invention relates to such compounds as isolated from their natural environment, preferably identifiable by aid of the novel coordinates defining structures according to the invention, as exemplified by the complementary compounds used in the complexes shown in Tables 9-11.

In a first embodiment, the present complementary compound is substantially complementary to an enzymatically active site of the protein and is advantageously capable of specifically inhibiting an enzymatic activity of said protein. Thus, in one embodiment, the present compound is substantially complementary to parts, or all, of the "basic" aminopeptidase binding site defined in Table 2 above. Thus, the present compound is an inhibitor capable of specifically inhibiting an aminopeptidase activity of an enzyme, preferably of LTA<sub>4</sub> hydrolase. In an alternative embodiment, the present compound is substantially complementary to parts, or all, of the leukotriene binding site as defined in Table 3 above. Thus, the present compound is an inhibitor capable of specifically inhibiting an epoxide hydrolase activity of an enzyme, preferably of LTA<sub>4</sub> hydrolase. (The inhibition of both aminopeptidase and epoxidase hydrolase is discussed in detail below in the experimental section.) As the present two binding sites of LTA<sub>4</sub> hydrolase overlap in part, a further embodiment is a compound which is complementary to essential parts



of both of the above discussed two binding sites, in part or partially, which thus preferably is an inhibitor of both the discussed activities.

As already mentioned above, one compound which is complementary to an enzymatically active site of LTA<sub>4</sub> hydrolase is a compound complementary to the M1 region thereof and thus capable of partial or total inhibition of the enzymatic activity of LTA<sub>4</sub> hydrolase or any other metallohydrolase belonging to the M1 family. In the present application, such inhibitors will be denoted M1 inhibitors.

As the skilled in this field will realise, the present inhibitors disclosed above need not be compound that inhibit a biological activity completely, but may be capable of exerting a partially inhibiting activity, i.e., lowering the enzymatic activity.

In another embodiment, the present complementary compound is a compound which is also capable of binding to the receptor for the product of an LTA<sub>4</sub> hydrolase, i.e. an LTB<sub>4</sub> receptor, e.g. on a cell, such as a polymorphonuclear leukocyte. Thus, such a compound may be useful as an LTB<sub>4</sub> antagonist whereby the biological effect of LTA<sub>4</sub> hydrolase activity may be regulated. Accordingly, any such LTB<sub>4</sub> antagonist designed and/or identified using the coordinates of LTA<sub>4</sub> hydrolase as presented herein are also encompassed by the present invention.

In another embodiment, the present complementary compound is a compound which, apart from being capable of binding to an active site of LTA<sub>4</sub> hydrolase, is also capable of binding to an active site of LTC<sub>4</sub> synthase which binds the same substrate as LTA<sub>4</sub> hydrolase, i.e. LTA<sub>4</sub>, and turns it over into LTC<sub>4</sub> (*cf.* Fig 1) and is thus expected to share important structural features with the active site of LTA<sub>4</sub> hydrolase. Such a compound may be useful as an inhibitor of LTC<sub>4</sub> biosynthesis, whereby the production thereof may be regulated. Accordingly, any such LTC<sub>4</sub> synthase inhibitor, designed and/or identified using the coordinates of LTA<sub>4</sub> hydrolase, are also encompassed by the present invention.



The specific properties and advantageous uses of the present compounds as well as the design and production of novel LTA<sub>4</sub> hydrolase inhibitors will be described in further detail below in relation to the various methods.

#### 2.4.3 A complex of LTA<sub>4</sub> hydrolase and a complementary compound

In a third aspect, the present invention relates to an isolated complex comprised of a protein as described above and a compound complementary to said protein. Said complementary compound may thus be an inhibitor of one or more of the protein's enzymatic activities, such as an aminopeptidase and/or epoxide hydrolase activity, such as bestatin, hydroxamic acid or thiolamine, or leukotriene B<sub>4</sub> or any analogue thereof, or LTC<sub>4</sub> or any analogue thereof. Examples of complementary compounds are bestatin, thiolamine or hydroxamic acid. In the present context, it is to be understood that the invention also relates to specific regions of said inhibitors, that have never been specifically disclosed for the present purpose, as well as novel inhibitors identified by aid of the present invention. In specific embodiments, the complex according to the invention is composed of LTA<sub>4</sub> hydrolase complexed with bestatin, thiolamine or hydroxamic acid, respectively, as defined by the coordinates presented in Tables 9-11, or any functional fragment, derivative or analogue thereof. As bestatin is aminopeptidase based, further similar and advantageous inhibitors may be developed based on the structural information provided in Table 9, preferably combined with the specification of the binding site of Table 2. Further, as both thiolamine and hydroxamic acid are leukotriene based, the information provided in Tables 10 and 11, preferably combined with the specification of binding site of Table 3, will prove to be an advantageous tool in order to gain more information about such enzymatic binding and thus the development of further novel inhibitors.

Accordingly, the present invention presents for the first time the coordinates defining the three-dimensional structure of a complex of LTA<sub>4</sub> hydrolase and an inhibitor thereof as determined by X-ray crystallography and illustrated in Tables 9-



11. In fact, this is the first time ever to disclose any three-dimensional structure of a protein component of the leukotriene cascade. Due to these novel reliable parameters, the complex as well as the components thereof are readily distinguished from the prior art. Together with biochemical and mutagenetic data, the novel structures will provide the basis for understanding the molecular mechanisms of the aminopeptidase and epoxide hydrolase activities, as well as the enzyme's suicide inhibition. Accordingly, the present invention will open a whole range of new possibilities as regards e.g. identification and/or design of novel biologically active molecules and methods of controlling said cascade, *in vivo* or *in vitro*. Consequently, novel advantageous drugs, such as medicaments for the treatment and/or prevention of inflammatory and/or allergic diseases, may be designed, as will be discussed in further detail below.

In the present context, it is to be understood that proteins according to the invention include the naturally occurring three dimensional forms thereof, separated and isolated from its natural environments, as well as any such protein, wherein deletions, additions and/or substitutions of the amino acid sequence have been made, provided that the three dimensional structure is substantially maintained, as the exerted biological activity is critically dependent upon the particular three-dimensional folding of the protein. The present invention also encompasses any derivative or conformational analogue of the above disclosed proteins, which has a three-dimensional structure essentially as disclosed above, or an effective part thereof having the biological activities discussed in detail below.

#### 2.4.4 Advantageous uses of LTA<sub>4</sub> hydrolase, complementary compounds and complexes thereof

A fourth aspect of the present invention is the use of a protein, a complementary compound or a complex according to the invention in drug design, such as in molecular modeling, direct structure-based design and/or combinatorial chemistry. Such methods will be disclosed in detail below. The drugs designed using the above



mentioned compounds may be suitable for the treatment and/or prevention of disorders involving acute and chronic inflammatory symptoms, said disorder being selected from the group consisting of arthritis, inflammatory bowel disease (IBD), psoriasis, chronic obstructive pulmonary disease (COPD), and acquired immune deficiency syndrome (AIDS). Further, such a drug may be used for the treatment and/or prevention of proliferative disorders, such as neoplasias and/or cancer. Alternatively, a drug may be designed which is effective for the treatment and/or prevention of an inflammatory and/or allergic disorders caused by the lethal factor of *Bacillus anthracis*, e.g. anthrax. However, the above mentioned diseases are exemplary and other diseases or conditions not mentioned herein may also be contemplated.

In a further aspect, the present invention relates to the use of a protein having a structure substantially as defined for the LTA<sub>4</sub> hydrolase of the invention, or a part, analogue or derivative thereof, for screening a compound for possible medicinal activity. In the pharmaceutical industry, new or known compounds are routinely screened for new uses employing a variety of known *in vitro* or *in vivo* screens. Often such screens involve complex natural substances and are consequently expensive to carry out, and the results may be difficult to interpret. However, the knowledge of the three-dimensional protein structure according to the invention allows a preliminary screening to be carried out on the basis of the three-dimensional structure of a region thereof, and the structural similarity of a molecule which is being screened. Such screening can conveniently be carried out using computer modelling techniques, which match the three-dimensional structure of the protein or part thereof with the structure of the molecule being screened. Potential agonist or inhibitor activity may be predicted. As a result, the production efficiency, bioavailability, immunogenicity, stability etc. may be favourably changed with respect to their therapeutic application.

As regards the above disclosed M1 inhibitors, these compounds will presumably find a broader field of application than the other novel inhibitors according to the



invention. Thus, the novel general M1 inhibitors are advantageously used e.g. in models to disclose in further detail other enzymatic pathways. Further, they may also be used in the above mentioned type of methods of drug design etc.

#### 2.4.5 Screening for LTA<sub>4</sub> hydrolase analogues

##### 2.4.5 (a) Method

Accordingly, in another aspect, the invention relates to a method for screening LTA<sub>4</sub> hydrolase analogues that mimic at least a part of the three dimensional structure of LTA<sub>4</sub> hydrolase, which comprises the steps of

- (a) producing a multiplicity of analogue structures of the LTA<sub>4</sub> hydrolase
- (b) selecting an analogue structure represented by a three-dimensional representation wherein the three-dimensional configuration and spatial arrangement of specific regions, preferably involved in ligand binding of said LTA<sub>4</sub> hydrolase, remain substantially preserved.

The coordinates used are general for LTA<sub>4</sub> hydrolase are essentially as illustrated in Tables 9-11, as defined by atom nos 1-4876.

More specifically, analogue structures of LTA<sub>4</sub> hydrolase may be screened by their ability to catalyze a particular reaction which may be monitored by chemical physical or immunological means. Furthermore, the analogue structure may be selected from its ability to produce receptor ligands or inhibitors of secondary reactions, which may be monitored directly, as exemplified above, via binding assays, enzyme assays, chemical assays, or functional bioassays.

Thus, in one embodiment, the invention relates to a method of screening, wherein one or more analogues exhibiting epoxide hydrolase activity, are screened for. Thus, such a method may be primarily based on the data of Table 10 and 11, wherein the binding of thiolamine and hydroxamic acid to LTA<sub>4</sub> hydrolase is shown, preferably combined with the information of Table 3 regarding the active site of LTA<sub>4</sub>







134, using the LTA4 hydrolase numbering scheme, is modified to an alanine, valine, a leucine and so forth.

Table 5: Mutations in the active site

|  |       |
|--|-------|
| Q134G/A/V/L/I/S/T/D/E/N/R/H/K/P/C/M/F/Y/W  | 5(1)  |
| Q136G/A/V/L/I/S/T/D/E/N/R/H/K/P/C/M/F/Y/W  | 5(2)  |
| A137G/V/L/I/S/T/D/E/N/Q/R/H/K/P/C/M/F/Y/W  | 5(3)  |
| Y267G/A/V/L/I/S/T/D/E/N/Q/R/H/K/P/C/M/F/W  | 5(4)  |
| G268A/V/L/I/S/T/D/E/N/Q/R/H/K/P/C/M/F/Y/W  | 5(5)  |
| G269A/V/L/I/S/T/D/E/N/Q/R/H/K/P/C/M/F/Y/W  | 5(6)  |
| M270G/A/V/L/I/S/T/D/E/N/Q/R/H/K/P/C/F/Y/W  | 5(7)  |
| E271G/A/V/L/I/S/T/D/N/Q/R/H/K/P/C/M/F/Y/W  | 5(8)  |
| V292G/A/L/I/S/T/D/E/N/Q/R/H/K/P/C/M/F/Y/W  | 5(9)  |
| H295/G/A/V/L/I/S/T/D/E/N/Q/R/K/P/C/M/F/Y/W | 5(10) |
| E296/G/A/V/L/I/S/T/D/N/Q/R/H/K/P/C/M/F/Y/W | 5(11) |
| H299G/A/V/L/I/S/T/D/E/N/Q/R/K/P/C/M/F/Y/W  | 5(12) |
| W311G/A/V/L/I/S/T/D/E/N/Q/R/H/K/P/C/M/F/Y  | 5(13) |
| F314G/A/V/L/I/S/T/D/E/N/Q/R/H/K/P/C/M/Y/W  | 5(14) |
| W315G/A/V/L/I/S/T/D/E/N/Q/R/H/K/P/C/M/F/Y  | 5(15) |
| E318G/A/V/L/I/S/T/D/N/Q/R/H/K/P/C/M/F/Y/W  | 5(16) |
| V322G/A/L/I/S/T/D/E/N/Q/R/H/K/P/C/M/F/Y/W  | 5(17) |
| F362G/A/V/L/I/S/T/D/E/N/Q/R/H/K/P/C/M/Y/W  | 5(18) |
| V367G/A/L/I/S/T/D/E/N/Q/R/H/K/P/C/M/F/Y/W  | 5(19) |
| L369G/A/V/I/S/T/D/E/N/Q/R/H/K/P/C/M/F/Y/W  | 5(20) |
| I372G/A/V/L/S/T/D/E/N/Q/R/H/K/P/C/M/F/Y/W  | 5(21) |
| P374G/A/V/L/I/S/T/D/E/N/Q/R/H/K/C/M/F/Y/W  | 5(22) |
| D375G/A/V/L/I/S/T/E/N/Q/R/H/K/P/C/M/F/Y/W  | 5(23) |
| A377G/V/L/I/S/T/D/E/N/Q/R/H/K/P/C/M/F/Y/W  | 5(24) |
| Y378G/A/V/L/I/S/T/D/E/N/Q/R/H/K/P/C/M/F/W  | 5(25) |
| P382G/A/V/L/I/S/T/D/E/N/Q/R/H/K/C/M/F/Y/W  | 5(26) |



Y383G/A/V/L/I/S/T/D/E/N/Q/R/H/K/P/C/M/F/W 5(27)

R563G/A/V/L/I/S/T/D/E/N/Q/H/K/P/C/M/F/Y/W 5(28)

More specifically, this embodiment relates to an analogue comprising any combination of at least two mutated amino acids, or any one of the above mentioned sequences of mutations, or any separate one amino acid mutation selected from the group consisting of sequences nos 1-9, 13-15, 17-24, 26 and 28, which are all novel mutations that have never been published before the present application. However, the other sequences not specified above are novel in the present context and thus such specific uses thereof are within the scope of the present invention.

Table 6: Mutations of the curved outside of the N-terminal domain

|     |                                       |       |
|-----|---------------------------------------|-------|
| R17 | G/A/V/L/I/S/T/D/N/E/Q/H/K/P/C/M/F/Y/W | 6(1)  |
| K19 | G/A/V/L/I/S/T/D/N/E/Q/R/H/P/C/M/F/Y/W | 6(2)  |
| H20 | G/A/V/L/I/S/T/D/N/E/Q/R/K/P/C/M/F/Y/W | 6(3)  |
| H22 | G/A/V/L/I/S/T/D/N/E/Q/R/K/P/C/M/F/Y/W | 6(4)  |
| R24 | G/A/V/L/I/S/T/D/N/E/Q/H/K/P/C/M/F/Y/W | 6(5)  |
| D28 | G/A/V/L/I/S/T/N/E/Q/R/H/K/P/C/M/F/Y/W | 6(6)  |
| T33 | G/A/V/L/I/S/D/N/E/Q/R/H/K/P/C/M/F/Y/W | 6(7)  |
| T35 | G/A/V/L/I/S/D/N/E/Q/R/H/K/P/C/M/F/Y/W | 6(8)  |
| G36 | A/V/L/I/S/T/D/N/E/Q/R/H/K/P/C/M/F/Y/W | 6(9)  |
| T37 | G/A/V/L/I/S/D/N/E/Q/R/H/K/P/C/M/F/Y/W | 6(10) |
| A39 | G/V/L/I/S/T/D/N/E/Q/R/H/K/P/C/M/F/Y/W | 6(11) |
| T41 | G/A/V/L/I/S/D/N/E/Q/R/H/K/P/C/M/F/Y/W | 6(12) |
| Q43 | G/A/V/L/I/S/T/D/N/E/R/H/K/P/C/M/F/Y/W | 6(13) |
| K63 | G/A/V/L/I/S/T/D/N/E/Q/R/H/P/C/M/F/Y/W | 6(14) |
| V65 | G/A/L/I/S/T/D/N/E/Q/R/H/K/P/C/M/F/Y/W | 6(15) |
| N67 | G/A/V/L/I/S/T/D/E/Q/R/H/K/P/C/M/F/Y/W | 6(16) |
| N97 | G/A/V/L/I/S/T/D/E/Q/R/H/K/P/C/M/F/Y/W | 6(17) |
| E99 | G/A/V/L/I/S/T/D/N/Q/R/H/K/P/C/M/F/Y/W | 6(18) |



|      |                                       |       |
|------|---------------------------------------|-------|
| V101 | G/A/L/I/S/T/D/N/E/Q/R/H/K/P/C/M/F/Y/W | 6(19) |
| E103 | G/A/V/L/I/S/T/D/N/Q/R/H/K/P/C/M/F/Y/W | 6(20) |
| S105 | G/A/V/L/I/T/D/N/E/Q/R/H/K/P/C/M/F/Y/W | 6(21) |
| E107 | G/A/V/L/I/S/T/D/N/Q/R/H/K/P/C/M/F/Y/W | 6(22) |
| K153 | G/A/V/L/I/S/T/D/N/E/Q/R/H/P/C/M/F/Y/W | 6(23) |
| T155 | G/A/V/L/I/S/D/N/E/Q/R/H/K/P/C/M/F/Y/W | 6(24) |
| T157 | G/A/V/L/I/S/D/N/E/Q/R/H/K/P/C/M/F/Y/W | 6(25) |
| E159 | G/A/V/L/I/S/T/D/N/Q/R/H/K/P/C/M/F/Y/W | 6(26) |
| S161 | G/A/V/L/I/T/D/N/E/Q/R/H/K/P/C/M/F/Y/W | 6(27) |
| D175 | G/A/V/L/I/S/T/N/E/Q/R/H/K/P/C/M/F/Y/W | 6(28) |
| E177 | G/A/V/L/I/S/T/D/N/Q/R/H/K/P/C/M/F/Y/W | 6(29) |
| T178 | G/A/V/L/I/S/D/N/E/Q/R/H/K/P/C/M/F/Y/W | 6(30) |
| D180 | G/A/V/L/I/S/T/N/E/Q/R/H/K/P/C/M/F/Y/W | 6(31) |
| R186 | G/A/V/L/I/S/T/D/N/E/Q/H/K/P/C/M/F/Y/W | 6(32) |
| I188 | G/A/V/L/S/T/D/N/E/Q/R/H/K/P/C/M/F/Y/W | 6(33) |
| K190 | G/A/V/L/I/S/T/D/N/E/Q/R/H/P/C/M/F/Y/W | 6(34) |
| I192 | G/A/V/L/S/T/D/N/E/Q/R/H/K/P/C/M/F/Y/W | 6(35) |
| K194 | G/A/V/L/I/S/T/D/N/E/Q/R/H/P/C/M/F/Y/W | 6(36) |

Table 7: Mutations at the proline rich region

|      |  |      |
|------|--|------|
| T359 | G/A/V/L/I/S/D/N/E/Q/R/H/K/P/C/M/F/Y/W  | 7(1) |
| E358 | G/A/V/L/I/S/T/D/N/Q/R/H/K/P/C/M/F/Y/W  | 7(2) |
| D443 | G/A/V/L/I/S/T/N/E/Q/R/H/K/P/C/M/F/Y/W  | 7(3) |
| A446 | G/V/L/I/S/T/D/N/E/Q/R/H/K/P/C/M/F/Y/W  | 7(4) |
| Y449 | G/A/V/L/I/S/T/D/N/E/Q/R/H/K/P/C/M/F/W  | 7(5) |
| S450 | G/A/V/L/I/T/D/N/E/Q/R/H/K/P/C/M/F/Y/W  | 7(6) |
| P451 | G/A/V/L/I/S/T/D/N/E/Q/R/H/K/C/M/F/Y/W  | 7(7) |
| G452 | /A/V/L/I/S/T/D/N/E/Q/R/H/K/P/C/M/F/Y/W | 7(8) |
| L453 | G/A/V/I/S/T/D/N/E/Q/R/H/K/P/C/M/F/Y/W  | 7(9) |



|  |       |
|--|-------|
| P454 G/A/V/L/I/S/T/D/N/E/Q/R/H/K/C/M/F/Y/W | 7(10) |
| P455 G/A/V/L/I/S/T/D/N/E/Q/R/H/K/C/M/F/Y/W | 7(11) |
| I456 G/A/V/L/S/T/D/N/E/Q/R/H/K/P/C/M/F/Y/W | 7(12) |
| K457 G/A/V/L/I/S/T/D/N/E/Q/R/H/P/C/M/F/Y/W | 7(13) |
| P458 G/A/V/L/I/S/T/D/N/E/Q/R/H/K/C/M/F/Y/W | 7(14) |
| N459 G/A/V/L/I/S/T/D/E/Q/R/H/K/P/C/M/F/Y/W | 7(15) |
| Y460 G/A/V/L/I/S/T/D/N/E/Q/R/H/K/P/C/M/F/W | 7(16) |
| D461 G/A/V/L/I/S/T/N/E/Q/R/H/K/P/C/M/F/Y/W | 7(17) |

#### 2.4.5 (d) Nucleic acids encoding the novel compounds

Further, the invention also relates to an isolated nucleic acid encoding a novel analogue as defined above, that is, including a combination of any at least two of said mutations or one of the novel mutations, as well as a nucleic acid capable of specifically hybridising to a such a nucleic acid. The conditions of specific hybridisation are defined above in the section "Definitions". Further, the invention also relates to any vector or carrier comprising such a nucleotide, such as plasmids, viral vectors, e.g. retrovirus, oligonucleotides etc. Thus, any cell including such a nucleic acid or vector are also within the scope of the present invention and may e.g. be a mammalian cell, such as a human cell, or any other eucaryotic cell, or a procaryotic cell, such as a bacterium. The above mentioned elements may be used in the design of model systems useful in the study of the diseases discussed elsewhere in this application, which systems may be cell cultures, animal models, such as mice, etc.

#### 2.4.6 (a) Production and purification of genetically modified forms of LTA<sub>4</sub> hydrolase

Yet another aspect of the present invention is a process for the production of a novel genetically modified form of LTA<sub>4</sub> hydrolase identified or designed according to the present invention. Thus, the present process involves, after conventional steps of insertion a gene encoding the desired product in a host cell and expression thereof, a purification procedure, which includes a hydroxyapatite-based chromatography and



a subsequent anion exchange chromatography. These last two steps have been shown to be especially advantageous, in fact, even crucial, for obtaining a satisfying purity of the novel LTA<sub>4</sub> hydrolase forms according to the invention. The preceding steps are conventional as disclosed in literature and are easily performed by the skilled in this field.

Thus, in more detail, the invention relates to a method for purification of LTA<sub>4</sub> hydrolase comprised of (i) precipitation with ammonium sulphate, followed by (ii) separations on FPLC using anion exchange, hydrophobic interaction, and chromatofocusing resins, essentially as described (Wetterholm A., Medina J.F., Rådmark O., Shapiro R., Haeggström J.Z., Vallee B.L., Samuelsson B. *Biochim. Biophys. Acta.* 1080, 96-102 (1991)). To achieve a purity suitable for crystallography, we used (iii) chromatography on hydroxyapatite, e.g., on a TSKgel HA-1000, Tosohaas, followed by (iv) a step of anion-exchange chromatography on e.g., Mono-Q HR5/5.

Further, example 4 below describes in detail a purification of LTA<sub>4</sub> hydrolase according to the invention. Said example may be generalised to describe further the purification according to the invention.

#### 2.4.6 (b) Purified LTA<sub>4</sub> hydrolase

Further, the invention also relates to an essentially pure form of LTA<sub>4</sub> hydrolase obtained by the process described above.

#### 2.4.7 Screening for LTA<sub>4</sub> hydrolase binding compounds

##### 2.4.7 (a) Method

In yet a further aspect, the present invention relates to a method for screening LTA<sub>4</sub> hydrolase binding compounds complementary to a region, preferably an enzymatically active site, e.g. as defined in Tables 1-3, of the LTA<sub>4</sub> hydrolase molecule, which comprises the steps of

(a) producing a multiplicity of possible complementary structures and



(b) selecting a structure represented by a three-dimensional representation, wherein the three-dimensional configuration and spatial arrangement of regions of LTA<sub>4</sub> hydrolase involved in binding remain substantially preserved, which selection is based on the three-dimensional structure of LTA<sub>4</sub> hydrolase and/or LTA<sub>4</sub> hydrolase complexed to an inhibitor thereof, as defined by the coordinates of Table 9, 10 or 11.

More specifically, the method according to the invention will advantageously be used to select compounds capable of inhibiting epoxide hydrolase activity and/or aminopeptidase activity, LTB<sub>4</sub> receptor antagonists or inhibitors of LTC<sub>4</sub> synthases or inhibitors of any member of the M1 class of metallohydrolases. In one preferred embodiment, general enzyme inhibitors are screened for, which inhibitors are useful in the control of any one of a plurality of enzymatic pathways, wherein a metallohydrolase of the M1 type is participating. These general metallohydrolase inhibitors are herein denoted M1 inhibitors.

#### *Structure-based design of inhibitors*

In a further embodiment, the present invention relates to a method of structure-based design of LTA<sub>4</sub> hydrolase inhibitors. Such methods are based on the use of the present coordinates, or preferably the coordinates defining a selected region, as templates in order to synthesize advantageous inhibitors with strong and specific binding properties. More specifically, said method first uses a conventional organic synthesis, alone or combined with combinatorial chemistry, wherein the structure of the product of the synthesis is then further refined by cycles of crystallisation of enzyme and inhibitor, followed by another chemical synthesis, the product of which is again refined, etc.

Example 2 describes such a design, wherein it is noted that the removal of an extra carbon atom could yield a compound, which is a better inhibitor than this hydroxamic acid compound. Thus, similar conclusions will be drawn from the present method and result in inhibitors with superior properties compared to any prior art inhibitors.



#### 2.4.7 (b) Identified binding compounds

Further, the present invention also relates to any novel compounds identifiable by the present method. Advantageous and desired properties as well as other features of such compounds, e.g. as inhibitors, is discussed above in relation to complementary compounds, analogues etc. In one preferred embodiment of the invention, such an identified compound is an inhibitor of another M1 enzyme than LTA<sub>4</sub> hydrolase, such as . The medicinal aspects of the present compounds will be discussed below.

#### 2.4.8 Protein engineering

##### 2.4.8 (a) Method

In a further aspect, the present invention relates to a method of engineering a protein, which method comprises the steps of

- identification of a suitable set of mutation sites based on the structure of LTA<sub>4</sub> hydrolase according to the invention,
  - generation of a library of genes which contains the suitable sequence variations;
  - selection of clones encoding a LTA<sub>4</sub> analogue with a desired activity;
- wherein said desired activity is the capability of efficiently producing organic compounds of interest.

The present method is based on recent techniques available for generating large libraries of mutated genes (>1 billion variants) which can be attributed to a selection process of individual genes in the laboratory. Such directed evolution schemes have enormous potential for the design of new proteins, including new substrate specificity for enzymes as well as improving enzyme activities.

Directed evolution, or combinatorial engineering schemes have been successfully applied in evolving RNA molecules with improved binding and catalytic activities (Lorsch and Szostak, 1994). Also binding proteins (and peptides) with good affinities can now routinely be evolved based on a range of different protein folds (Nord et al, 1997). The present methods may be used to perform such a directed







In an advantageous embodiment, the present method is used to engineer LTA<sub>4</sub> hydrolase inhibitors and/or analogues. In a specific embodiment of said method, a compound capable of mimicking the suicidal mode of LTA<sub>4</sub> hydrolase catalysis, thus acting as a mechanism-based suicide inhibitor, or otherwise capable of regulating the production of LTB<sub>4</sub> is engineered. In an alternative embodiment, an inhibitor of LTC<sub>4</sub> synthase or an LTB<sub>4</sub> receptor antagonist is designed.

#### 2.4.8 (b) Novel specifically designed proteins

Further, the present invention also relates to any novel protein designed by use of the above described method. Once specified, such proteins may be produced by any conventional method well known to the skilled in this field, some of which are exemplified below. In Example 2 below, the binding of hydroxamic acid to LTA<sub>4</sub> hydrolase is discussed. Thus, such a modified hydroxamic is one example of a novel inhibitor specifically designed according to the invention, and the reasoning in the example may be used as a basis for the way of reasoning that is used in the present design.

Accordingly, novel enzymes may be produced, which are capable of any different chemical activity. For example, enzymes capable of novel catalytic properties, enzymes that in turn produce enzymes, etc., may be produced according to the present invention.

#### 2.4.8 (c) Use of genetically modified LTA<sub>4</sub> hydrolase

The invention also encompasses the use of a genetically modified LTA<sub>4</sub> hydrolase, obtained by any method according to the invention, with altered catalytic properties, e.g., increased ability to synthesize LTB<sub>4</sub>. The modified enzyme may thus be used for production of LTB<sub>4</sub>, or any analogues substances, a biomedical reagent which in turn may be used in, e.g., studies of leukotriene metabolism, induction of chemotaxis, as a reference compound in analysis of leukotrienes etc.

#### 2.4.9 Pharmaceutical applications of the present invention



#### 2.4.9 (a) First medical indication

Further, the invention also encompasses a compound obtainable by the method of screening LTA<sub>4</sub> hydrolase binding compounds or the protein engineering methods described above, and more preferably, said compound for use as a medicament. One specifically advantageous embodiment is the herein disclosed novel M1 inhibitor for use as a medicament.

In an advantageous embodiment, the present compounds are used in the manufacture of a medicament for the treatment and/or prevention of acute and chronic inflammatory disorders, said disorder being selected from the group consisting of arthritis, inflammatory bowel disease (IBD), psoriasis and chronic obstructive pulmonary disease (COPD); neoplasias and/or cancer; or disorders caused by the lethal factor of *Bacillus anthracis*, e.g. anthrax. Alternatively, the use may relate to the manufacture of a medicament for the treatment and/or prevention of an inflammatory and/or allergenic disorder, such as bronchial asthma, allergic rhinitis, conjunctivitis etc. Yet an alternative use is in the manufacture of a medicament for the treatment and/or prevention of infection caused by human immunodeficiency virus (HIV). The novel M1 inhibitor are preferably used in medicaments for the treatment and/or prevention of such various diseases as cancer and/or endocrinological disturbances.

#### 2.4.9 (b) Second medical indication and pharmaceutical methods

Thus, the present invention relates to the above mentioned molecules prepared by the method according to the invention for use in the manufacture of various medicaments for the above defined conditions. The invention also encompasses pharmaceutical preparations containing these molecules together with pharmaceutically acceptable carriers. Methods for the preparation of pharmaceutical preparations are e.g. found in Remington's Pharmaceutical Sciences, Mack Publishing Company, Philadelphia, PA, 17<sup>th</sup> ed. (1985). For a review of drug delivery, see Langer, Science 249:1527-1533 (1990). As those skilled in this field



easily realise, the form of such a pharmaceutical preparation, the mode of administration thereof as well as suitable dosages will depend on the specific disease to be treated, the nature of the active substance used, the patient's age, body weight etc.

#### 2.4.9 c) Methods of treatment

The present invention also encompasses any method of treatment for the above defined purposes. Exact details regarding such methods are determined by the practitioner depending on the specific circumstances from case to case.

#### 2.5 Production of novel molecules

The compounds, which may be proteins, polypeptides, peptides or any other organic molecules, prepared according to the methods according to the invention may be synthesized chemically by methods well known to those of skill in this field or they may be prepared by use of recombinant DNA technology by any suitable method well known to those of skill in this field. General methods of synthesis are e.g. found in Berger and Kimmel, Guide to Molecular Cloning Techniques, Methods in Enzymology, vol. 152, Academic Press, Inc., San Diego, CA; Sambrook et al., Molecular Cloning, A Laboratory Manual, 2<sup>nd</sup> Ed., vol. 1-3, Cold Spring Harbor Laboratory, Cold Spring Harbor, NY, 1989; and Current Protocols in Molecular Biology, F.M. Ausbel et al., Current Protocols (1994). Methods of reducing and denaturing proteins and inducing re-folding are well known to those of skill in the art, see e.g. Debinski et al., J. Biol. Chem., 268: 14065-14070 (1993); Kreitman and Pastan, Bioconjug. Chem., 4: 581-585 (1993); and Buchner et al., Anal. Biochem., 205: 263-270 (1992).

#### 2. 6 Detailed description of the drawings

Figure 1 shows key enzymes and intermediates in leukotriene biosynthesis.

Figure 2 shows 2Fo-Fc density contoured at 1.1  $\sigma$ . Part of the active site in the neighborhood of the bestatin molecules is shown. Figures are created using a modified version of Molscript48,49.



Figure 3 is a ribbon diagram of the tertiary structure of LTA4 hydrolase. The N-terminal domain at the top of the diagram is rich in  $\beta$ -strands and connects to the catalytic domain to the left in the figure which is more  $\alpha$ -helical and extends into the central part of the molecule. The C-terminal domain, illustrated at the bottom of the ribbon diagram, extends towards the right side of the catalytic domain.

Figure 4 (a) is a ribbon diagram of the N-terminal domain with its layers of  $\beta$ -strands, while (b) is a superimposition of the  $C\alpha$  trace of the N-terminal domain on the  $C\alpha$  trace of bacteriochlorophyll *a*. The N-terminal domain covers approx. half of the bacteriochlorophyll *a* structure (the right and bottom part of the diagram).

Figure 5 (a) is a ribbon diagram of the catalytic domain. In the center of the diagram, the three zinc binding ligands, His295, His299, and Glu318, as well as the inhibitor bestatin are depicted in ball and stick representation. The zinc ion is shown as a CPK model. The diagram in (b) shows the structure of thermolysin in the same orientation as the catalytic domain of LTA4 hydrolase. The three zinc ligands, His142, His146, and Glu166, as well as the inhibitor Cbz-GlyP-(O)-Leu-Leu50 are depicted in ball-and stick representation. The zinc ion is shown as a CPK model.

Figure 6 shows the structure of the C-terminal domain.

Figure 7 shows the zinc binding ligands in LTA4 hydrolase, His295, His299, and Glu318, superimposed on those in thermolysin, His142, His146, and Glu-166. Other catalytic or neighboring residues in the two enzymes are Tyr383, Glu325, Glu296, Thr302, and Asn317 in LTA4 hydrolase which correspond to His231, Asp170, Glu143, Asn165, and Tyr157 in thermolysin.

Figure 8 (a) is a Ball-and-Stick presentation of the binding of bestatin in LTA4 hydrolase.

Figure 8 (b) is a schematic overview of bestatin binding in LTA4 hydrolase.

Figure 9 (a) is a wire representation of the cavity found in LTA4 hydrolase (shown as  $C\alpha$ -trace).

Figure 9 (b) is a schematic presentation for the proposed binding of LTA4 into the cavity.



Figure 10 is a schematic representation for the proposed epoxide hydrolase reaction mechanism. The catalytic zinc acts as a Lewis acid and activates the epoxide to form a carbocation intermediate according to an  $S_N1$  reaction. Water is added at C12 in a stereospecific manner, presumably directed by Asp375. The double bond geometry is controlled by the binding conformation of LTA4. Further details are given elsewhere in the present description.

### 3. EXPERIMENTAL

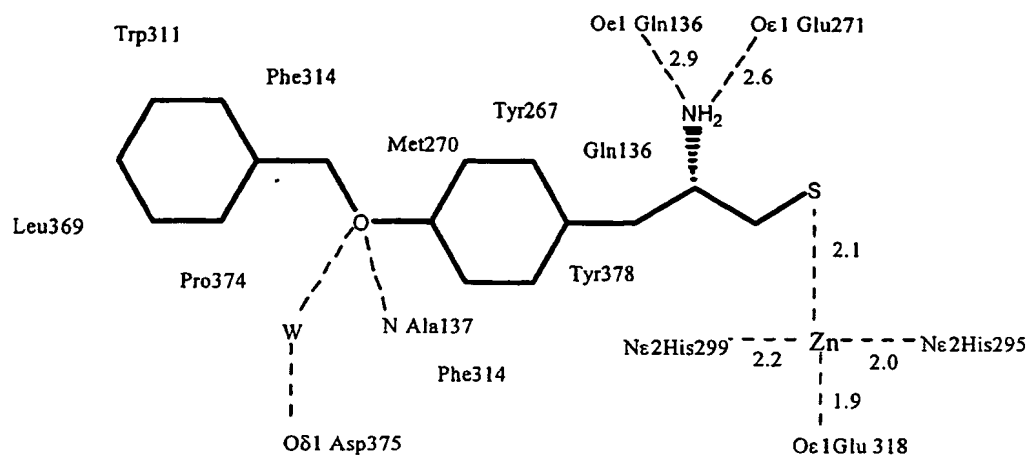
The following examples are intended for illustrating purposes only and should not in any way be used to construe the scope of the protection of the present invention as defined by the appended claims. All the references given below, and previously in this specification, are hereby included herein by reference.

#### 3.1 Examples

##### Example 1: Binding of the thiol-compound (I)

The thiol group of the compound is ligated to the  $Zn^{2+}$  ion, that has a tetra-hedral configuration. Both the phenyl-groups are making extensive hydrophobic interactions. The first one makes aromatic stacking interactions with Phe314 and Trp311. Further hydrophobic interactions are made with Pro374 and Leu369. The other phenyl ring is making stacking interactions with Tyr267 and Tyr378. Met270 and Gln136 provide additional hydrophobic interactions. The ether-oxygen in the linker between the two phenyl rings makes a hydrogen bond to the backbone nitrogen of Ala137 and also with a water molecule which is linked to Asp375. The amine group makes interactions to the O $\epsilon$ 1 of Gln136 and the O $\epsilon$ 1 of Glu271.





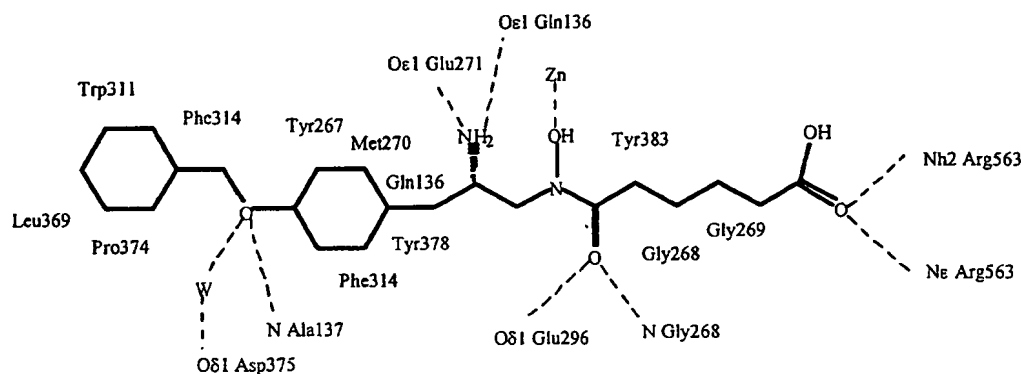
Formula (I)

### Example 2: Binding of the hydroxamic acid compound (II)

The binding of this compound is very similar to the binding of the thiol compound described above. The manner in which the phenyl-moieties, the linker region and the amine group are bound is identical. The manner in which the hydroxamic acid part is bound is different in comparison with other complexes such as thermolysin-HA complexes and LTA<sub>4</sub>-hydrolase-bestatin complex. Instead of a double interaction of the hydroxyl and carbonyl oxygens and the Zn ion resulting in a pentavalent co-ordination, here only one of the oxygens (the hydroxyl) is making an interaction with the Zn ion giving a tetrahedral co-ordination. The other oxygens make an interaction to Asp296 and the backbone nitrogen of Gly268. This difference is probably due to the tight binding of the phenyl rings and the amine group. The linkage between the amine group and the hydroxamic acid group contains one more carbon atom than in a normal or modified peptide-linkage. Since the binding site for substrates is rather narrow near the Zn ion, the conformation of compounds which bind in this area is rather restricted. Therefore one of the otherwise binding oxygens is pushed out and can no longer make an interaction with the Zn<sup>2+</sup> ion. Removal of this extra carbon atom could yield a compound which is a better inhibitor than this



hydroxamic acid compound. The acid group at the other end of the compound is fixed by making a double interaction with the N $\epsilon$  and the Nh2 of Arg563.



Formula (II)

### Example 3: Structure determination of two specific inhibitor-LTA<sub>4</sub> hydrolase complexes

Crystals, grown as described above, were soaked in 1 mM solution of thiolamine (Yuan et al., 1993) or 0.5 mM solution of hydroxamic acid (Hogg et al., 1995) in 15% PEG8000, 50 mM Imidazol pH 6.7, 25 mM acetate and 2.5 mM YbCl<sub>3</sub>. After at least 24 hours, the crystals were transferred to a solution that contained a cryoprotectant (see above) and subsequently flash frozen in liquid nitrogen. The data for the crystal soaked with thiolamine was obtained at BM14B at the EMBL-outstation in DESY, Hamburg. The data for the hydroxamic acid was collected at beamline 7/11 at MAX-lab, Lund. Statistics from the data collections are shown in the table. The data were processed using MOSFLM, merging and other manipulations were performed by programs from CCP4 and the BIOMOL packages. The refinement procedures for both datasets were very similar. First rigid body refinement using TNT was performed. As a starting model for refinement and model building the structure of LTA<sub>4</sub> hydrolase complexed with bestatin was used.



The bestatin molecule and all water molecules were deleted from the model. After this initial refinement it was possible to build the inhibitors into the protein. For evaluation of the density maps and model-building the program QUANTA (Molecular Simulations Inc., Burlington, MA) was used. The refinement was continued using TNT and was combined with sessions of model-building. In all rounds no sigma cut-offs were used and the resolution was slowly increased during the procedure. Water molecules were identified and incorporated into the models. During these procedures the  $R_{\text{free}}$  was carefully monitored. When refinement had converged, it was finished with one round in which all reflections, including those who were used for the calculations of the  $R_{\text{free}}$ , were incorporated. Statistics about refinement and quality of the models can be found in Table 5.

Table: Statistics of refinement and quality of the model

|                 | Thiolamine (Thiol) | Hydroxamic acid (HA) |
|-----------------|--------------------|----------------------|
| Resolution      | 15-2.5Å            | 15-1.8Å              |
| Rfactor         | 17.8%              | 24.2%                |
| Rfree           | 24.4               | 29.7%                |
| Bond Lengths    | 0.011Å             | 0.012Å               |
| Angles          | 1.9°               | 2.0°                 |
| Trigonal groups | 0.005Å             | 0.006Å               |
| Planar groups   | 0.009Å             | 0.010Å               |
| Contacts        | 0.026Å             | 0.041Å               |
| No. of waters   | 252                | 127                  |

Example 4: Purification of LTA<sub>4</sub> hydrolase.



For adsorption chromatography on hydroxyapatite, a TSKgel HA-1000 column (Tosohaas) was equilibrated in 10 mM potassium phosphate buffer, pH 7.1, supplemented with 0.2 mM CaCl<sub>2</sub>. The enzyme sample was applied and a linear gradient of increasing phosphate (10 - 400 mM) was developed by mixing the starting buffer with 400 mM potassium phosphate buffer, pH 6.8, supplemented with 10 µM CaCl<sub>2</sub>. Active fractions containing LTA<sub>4</sub> hydrolase were eluted between 150 - 190 mM potassium phosphate.

Anion exchange chromatography was performed on a Mono-Q HR 5/5 column (Pharmacia Biotech) equilibrated with the loading buffer 10 mM Tris-Cl, pH 8. The pure protein was eluted using a linear gradient of KCl (0 - 500 mM) and was recovered at 110 - 140 mM KCl.

#### Example 5: Enzyme engineering

The present inventors have shown, that when Tyr-378 in LTA<sub>4</sub> hydrolase was exchanged for a Phe residue, the resulting mutated enzyme was no longer suicide inhibited by LTA<sub>4</sub> and exhibited a substantially increased catalytic efficiency. Furthermore, the mutated enzyme was capable of converting LTA<sub>4</sub> not only into the natural product LTB<sub>4</sub>, but also into a novel metabolite, 6-*trans*-8-*cis*-LTB<sub>4</sub>. (Mueller, M.J., *et al. Proc Natl Acad Sci U S A* 93, 5931-5935 (1996)).

#### Example 6: Enzyme-engineering

Tyr-383 in mouse LTA<sub>4</sub> hydrolase was exchanged for Gln residue, which resulted in a mutated enzyme capable of forming the unnatural product 5S, 6S-dihydroxy-7,9-*trans*-11,14-*cis*-eicosatetraenoic acid from LTA<sub>4</sub> (Andberg, M., Hamberg, M. & Haeggstrom, J.Z. *J. Biol. Chem.* 272, 23057-23063 (1997)).

#### Example 7: Crystallisation of LTA<sub>4</sub> hydrolase



LTA<sub>4</sub> hydrolase was crystallised using YbCl<sub>3</sub> as an additive, 15% PEG and 50 mM Na-acetate as precipitant and 50 mM imidazole, pH 6.7, as buffer. Liquid-liquid-diffusion in capillaries were used as crystallisation set-ups.

### 3.2 Materials and Methods

*Enzyme purification.* Human recombinant LTA<sub>4</sub> hydrolase was expressed in *E. coli* and purified to homogeneity in four chromatographic steps on FPLC using anion exchange, hydrophobic interaction, chromatofocusing, and hydroxyapatite resins, essentially as described (Wetterholm A., Medina J.F., Rådmark O., Shapiro R., Haeggström J.Z., Vallee B.L., Samuelsson B. Recombinant mouse leukotriene A<sub>4</sub> hydrolase: a zinc metalloenzyme with dual enzymatic activities. *Biochim. Biophys. Acta.* **1080**, 96-102 (1991)).

*Crystallization conditions.* The chemicals used for the crystallization experiments were purchased from Merck and were of highest purity available. The sparse matrix kit was obtained from Hampton Research. Crystallization conditions for the protein were initially sought by using the sparse matrix approach (Jancarik, J. & Kim, S.-H. J. Appl. Crystallogr. **24**, 409-411 (1991)) in hanging drop vapor diffusion set-ups in cell culture plates at room temperature. Under condition 28, (30% PEG8000, 0.2 M sodium-acetate, 0.1 M cacodylate buffer, pH 6.5) needles grew. They were subsequently reproduced and optimized using a finer grid search, different temperatures for the equilibration and testing of additives. Crystals were only obtained when the inhibitor bestatin was present in the crystallization set-ups. Using YbCl<sub>3</sub> as an additive and switching to liquid-liquid diffusion in capillaries, allowed plate-like crystals to grow. Thus, 5 µl 28% PEG8000, 0.1 mM Na-acetate, 0.1 mM imidazole buffer, pH 6.8, 5 mM YbCl<sub>3</sub> is injected into the bottom of a melting point capillary and an equal volume of LTA<sub>4</sub> hydrolase (5 mg/ml) in 10 mM Tris-Cl, pH 8, supplemented with 1 mM bestatin, is layered on top. Finally, the capillary is closed and stored at 22°C. Crystals with an average size of 0.6 x 0.4 x 0.05 mm<sup>3</sup> appear in 3 to 4 weeks.



*Crystal properties.* The plate-like crystals diffract beyond 2Å using synchrotron radiation. They belong to space-group P21212 with cell dimensions  $a = 67.59 \text{ Å}$ ,  $b = 133.51 \text{ Å}$ ,  $c = 83.40 \text{ Å}$ ,  $a = b = c = 90^\circ$  at 100K. As a cryo-solution, a mixture of 15%PEG 8000, 50 mM Na-acetate, 50 mM imidazole buffer, pH 6.8, 2.5 mM YbCl<sub>3</sub>, and 25% glycerol was used. Assuming one molecule per asymmetric unit the solvent content of the crystals is 48%.

*Structure determination.* The structure was determined by using multiple anomalous dispersion measurements on the LIII edge of Ytterbium ( $\lambda = 1.3862 \text{ Å}$ ) at beam line BM14 at the European Synchrotron Radiation Facility (ESRF), Grenoble. Three datasets, peak (PK), point of inflection (PI) and remote (RM), were collected to 2.5Å resolution from the same crystal. The crystal was aligned such that Bijvoet equivalent reflections could be collected in one pass of  $90^\circ$  for each wavelength. For RM a subsequent dataset to 2.15Å was collected. A second crystal was used for obtaining a dataset to 1.95Å. (For statistics on data-collection and quality, see table 1). Data were integrated using the program Denzo, scaled to each other using Scalepack (Otwinowski, Z. *Data collection and Processing. Proceedings of the ccp4 study weekend. SERC Daresbury Laboratory, Warrington, UK.*, 56-62 (1993)) and further analyzed using programs from the CCP4 package (Collaborative Computing Project Number 4. *Acta Crystallogr. Sect. D* 50, 760-763 (1994)).

From Patterson functions one major and one minor Yb position could readily be identified, a third position was identified during heavy atom refinement in difference Fourier maps. The heavy atom parameters were refined using MLPHARE (Otwinowski, Z. *Isomorphous replacement anomalous scattering. Proceedings of the CCP4 study weekend. SERC Daresbury Laboratory, Warrington, UK.*, 80-85 (1991)) and SHARP (de La Fortelle, E. & Bricogne, G. *Met. Enzymol.* 276, 472-494 (1997)). The final figures of merit was 0.57 to 2.15Å. Phase information was further improved to 2.15Å by solvent flattening using SOLOMON (Abrahams, J.P. & Leslie, A.G.W. *Acta Crystallographica* D52, 30-42 (1996)) with a solvent content of



43%. The quality of the maps was very good and the entire protein molecule (residue 1-610) could be traced unambiguously. All model building was performed using QUANTA (Molecular simulations). Refinement was started by a run of slow-cooling molecular dynamics in XPLOR (Brünger, A.T., Kuriyan, J. & Karplus, M. *Science* 235, 458-460 (1987)) using the RM dataset to 2.7Å. The three Yb ions were included into the refinement with full occupancy for the first Yb and half occupancy for the two other ions. All subsequent refinement was performed with TNT (Tronrud, D.E., ten Eyk, L.F. & Matthews, B.W. *Acta Crystallogr. Sect. A* 43, 481-501 (1987)). The same set of reflections (4% of total amount from 25-1.95Å) for the calculation of  $R_{\text{free}}$  (Brünger, A.T. *Nature* 355, 472-475 (1992)) was maintained throughout all refinement procedures. The resolution was slowly improved by alternating sessions of model-building and refinement. The data for the second crystal to 1.95Å were used for further refinement during which a Zn ion, bestatin, an acetate and an imidazole molecule were identified. Judged from the B-factors these molecules are all fully occupied. 540 water molecules were added to the coordinates. The  $R_{\text{free}}$  was 24.7% and the working R-factor was 18.8% for all data between 25-1.95 Å. In a final round of refinement all data between 25-1.95 Å were included, yielding a final R-factor of 18.5 % for residues 1-610, 3 Yb ions, 1 Zn, 1 bestatin, 1 imidazole, 1 acetate and 540 water molecules. Most of the model is in good density (Fig. 2) except a loop encompassing residues 179 to 184 for which only poor density was obtained. The model has good stereo-chemical parameters (r.m.s bonds = 0.010Å, r.m.s angles = 2.2°) and 91.7% of the residues lie in the most favored part of the Ramachandran plot.

#### 4. RESULTS AND DISCUSSION

##### 4.1 Overall structure and domain organization

The leukotriene A<sub>4</sub> hydrolase molecule is folded into three domains; an N-terminal domain, a catalytic domain and a C-terminal domain which together form a flat triangular arrangement with approximate dimensions of 85 x 65 x 50 Å<sup>3</sup>. The overall structure of the enzyme is depicted in figure 3. Although the three domains pack closely and make contact with each other, a deep cleft is formed in between.



#### 4.2 The N-terminal domain is structurally related to bacteriochlorophyll *a*

The N-terminal domain (residue 1-209) is composed of one 7 stranded mixed  $\beta$ -sheet, one 4 and one 3 stranded antiparallel  $\beta$ -sheet. Strands from the larger  $\beta$ -sheet continue into the two smaller  $\beta$ -sheets that pack on the edges of the same side of the larger sheet so that a kind of envelope is formed (Fig. 4a & b). The two small  $\beta$ -sheets are turned towards the inside of the whole protein while the larger  $\beta$ -sheet is exposed to solvent and forms a large concave surface area. Loops connecting the other strands and hydrophobic residues fill the core of this domain. The N-terminal domain of LTA4 hydrolase shares important structural features with the chlorophyll-containing enzyme bacteriochlorophyll (Bchl) *a* (Matthews, B., Fenna, R., Bolognesi, M., Schmid, M. & Olson, J. *J. Mol. Biol.* **131**, 259-285 (1979)). Thus, 111 C $\alpha$  positions have equivalent positions in the two proteins despite the absence of any sequence identity (Fig. 4b). The domain is about half the size of Bchl *a* which has a single domain structure without major extensions. Like Bchl *a*, the shape of the N-terminal domain resembles an envelope (or Taco) with a hollow inside and in Bchl *a*, 7 bacteriochlorophylls are buried in this cavity. However, the domain is not as hollow as Bchl *a* since loop 135-155, which contains a small helical segment, is turned inwards and fills up the core. In Bchl *a* the equivalent loop (290-305) is positioned more towards the exterior of the protein, thereby leaving space for some of the tertrapyrroles of the bacteriochlorophylls. The large sheet (17 strands) of Bchl *a* is truncated to only 7 strands in LTA4 hydrolase. Especially the region between residue 35 and 263 of Bchl *a* has been replaced by a much shorter region in LTA4 hydrolase (res. 45 to 98) that forms the 3 stranded small  $\beta$ -sheet and the edge strand of the larger 7 stranded  $\beta$ -sheet. The structure of the other half of the molecule is almost completely conserved, except the insertion of two extra strands instead of loops in LTA4 hydrolase. The structural homology between Bchl *a*, a protein involved in light harvesting, and LTA4 hydrolase was certainly unexpected. In LTA4 hydrolase, the function of the N-terminal domain is not yet known, but one may speculate that it participates in binding to hydrophobic molecules or surfaces



with a possible regulatory function. In mammalian 15-lipoxygenase, a similar function was proposed for an N-terminal  $\beta$ -barrel domain with structural homology to a corresponding C-terminal domain in mammalian lipases (Gillmor, S.A., Villasenor, A., Fletcher, R., Sigal, E. & Browner, M.F. *Nature Struct. Biol.* 4, 1003-1009 (1997)).

The connection from the N-terminal to the catalytic domain is very short, a strand from the 4 stranded  $\beta$ -sheet connects into a strand of a 5-stranded anti-parallel  $\beta$ -sheet of the catalytic domain. The two sheets are closely packed and the interface is mainly hydrophobic in character with 14 hydrophobic residues contributing from the N-terminal domain and 11 from the catalytic domain. Hydrogen bonds occur between Gln116 and Ser264, Ser124 and Gln226, the backbone of Ser124 and Glu223, the backbone of Ser151 and Lys309, Lys153 and the backbone of Leu305 and indirectly through a water molecule between Tyr130 and the backbone of Val260. Two salt-bridges between His139 and Asp375 and between Arg174 and Asp257 complete the interactions made in this interface.

#### 4.3 The catalytic domain contains the zinc binding site and is structurally similar to thermolysin

The structure of the catalytic domain (res. 210-450) is surprisingly similar to the structure of thermolysin (Fig. 5a & b) (Holmes, M. & Matthews, B. *J. Mol. Biol.* 160, 623-639 (1982)). When the amino acid sequence in this domain was compared with that of thermolysin, the sequence identity was found to be very low (essentially confined to the zinc binding motifs). However, the structural homology stretches out over the whole domain. Thus, no less than 146 Ca positions overlap with an r.m.s. deviation of 1.946 Å. Like thermolysin, the catalytic domain consists of two lobes, one mainly  $\alpha$ -helical and one mixed  $\alpha$ /b lobe. The  $\alpha$ -lobe consists of 6 major helices interconnected by long loops containing smaller helical segments, while the  $\alpha$ /b lobe has a 5 stranded mixed  $\beta$ -sheet lined with 3 helices on one side. The zinc binding site is found in between the two lobes. Since this domain contains only 245 amino acids and thermolysin contains 314 residues, some truncations have taken place,



especially in the a/b lobe in which the N-terminal extended b structure is truncated and only a mixed 5 stranded  $\beta$ -sheet remains. The changes in the a-lobe are smaller. Here the long meandering loop 181 to 221 has been replaced by a long  $\alpha$ -helix and the b-hairpin from 245 to 258 has been deleted.

A loop in extended conformation on the surface of the protein from 451 to 463 connects the catalytic domain with the C-terminal domain. Interestingly, this segment contains a highly conserved proline rich motif P451-G-f-P-P-x-K-P-x-Y460 which bears some resemblance to an SH3 domain recognition sequence. However, the canonical arginine residue is not present on either side of the proline motif. Nevertheless, since this stretch of amino acids is exposed on the surface of the protein, it is still possible that it could serve as an anchoring site for protein-protein interactions.

The C-terminal domain (464-610) is composed of 9  $\alpha$ -helices that form an unusual coil of helices reminiscent of the ones found in lytic transglycosylase<sup>40</sup> and recently in the armadillo repeat region of b-catenin (Huber, A.H., Nelson, W.J. & Weis, W.I. *Cell* 90, 871-882 (1997)) (Fig. 6). The helices pack into two layers of parallel helices (5 inner and 4 outer helices) and in an anti-parallel manner between the two layers. The arrangements found in the two other proteins are much larger and form super-helical structures. In the C-terminal domain of LTA<sub>4</sub> hydrolase, the arrangement is more straight and has a very compact shape. One of the helices is deformed and one of the interconnecting loops is long and contains a small 310 helix. The domain makes contacts with both the a-lobe of the catalytic domain and one of the edges of the N-terminal domain. It is positioned in a way such that the helices lie perpendicular to the 7 stranded  $\beta$ -sheet of the N-terminal domain and to most of the helices in the catalytic domain. The helices are amphipathic in character, with the hydrophobic sides towards the middle of the domain and hydrophilic residues pointing towards the solvent and into the deep cleft in the middle of the



whole molecule. This side of the cleft is highly polar; 10 Arg and Lys residues and 4 Asp and Glu residues are positioned on this side.

#### 4.4 Zinc coordination

The immediate surroundings of the active site  $\text{Zn}^{2+}$  ion are very similar in thermolysin and LTA4 hydrolase. The  $\text{Zn}^{2+}$  is bound between the two lobes and is coordinated by His295, His299, one carboxylic oxygen of Glu318 and the carbonyl and hydroxyl oxygens of the inhibitor bestatin so that a square based pyramid is formed. The two histidines originate from a long  $\alpha$ -helix and the glutamate from a neighboring  $\alpha$ -helix, all in the  $\alpha$ -lobe. Glu296 and Tyr383, two residues implicated in the reaction mechanism for the peptide cleaving activity, are located near the Zn ion. Glu296, the putative general base, is positioned next to the metal ligand His295 and bends over the bestatin molecule and Tyr383, which was described as a proton donor, also makes contact with the bestatin molecule (Figure 8a).

Interestingly, the second layer around the Zn ion shows differences between thermolysin and LTA4 hydrolase. In both enzymes the orientation of the zinc binding ligands is fixed by hydrogen bonds, however the hydrogen bond acceptors are positioned differently. In thermolysin, the Nd1 of His142 is hydrogen bonded to the Od2 of Asp170, while in LTA4 hydrolase the Nd1 of His295 is hydrogen bonded to the Oe1 of Glu325. This residue comes from a structural equivalent to the helix carrying Asp170 in thermolysin, but is shifted half a turn outwards. The Nd1 of His146 in thermolysin is hydrogen bonded to the Od1 of Asn165. This residue is part of the zinc binding signature and is conserved between the two enzymes. However, in LTA4 hydrolase the helix in which this conserved residue is placed has been rotated slightly and Asn317 is no longer making a hydrogen bond to His299. The orientation of His299 is now fixed by a hydrogen bond from the Nd1 to the carbonyl backbone oxygen of Thr302. The Od1 of Asn317 makes instead a hydrogen bond to the backbone amide of Asn381 while the Nd2 makes a hydrogen bond to the hydroxyl group of Tyr200. The last protein-ligand, Glu166 is in



thermolysin hydrogen bonded to Tyr157 and a water molecule, in LTA<sub>4</sub> hydrolase, Glu318 is only hydrogen bonded to a water molecule (Fig. 7).

#### 4.5 Bestatin binding

Although the zinc binding site is formed by residues only from the catalytic domain and most catalytic residues also come from this domain, the active site itself is surrounded by loops from all three domains. The binding of bestatin reflects this, since it makes interactions with residues from all three domains. The main interactions of bestatin are made through the carbonyl and hydroxyl oxygens to the Zn atom. Hydrophobic interactions are made between the phenyl moiety and the phenyl rings of Tyr267, Phe316, Tyr378 and Tyr383. Also, Met270 and Gln136 are involved (Fig. 8a). The other end of the inhibitor is pointing towards the solvent, the leucine moiety makes interactions with Val292 and His295, while the carboxylic oxygens make interactions with Arg563 and Lys565 through water molecules as well as hydrogen bonds to the backbone nitrogen atoms of Gly268 and Gly269. Hydrogen bonds are formed between the peptidyl N of bestatin and Oe2 of Glu296 and between the terminal NH<sub>2</sub> and the Oe1 of Glu271 and Oe1 of Gln136. The hydroxyl oxygen makes apart from the interaction with the Zn ion also an interaction to the OH of Tyr383. (For schematic overview see Fig. 8b). Tyr378 which gets modified during suicide inactivation sits slightly further away, but makes a hydrogen bond to Tyr383 and some hydrophobic interactions with the phenyl ring of the inhibitor. These two tyrosine are both found on the same stretch of amino-acids that in thermolysin form a long a helix, however in leukotriene hydrolase this helix is interrupted and two turns of the helix are replaced by three residues (378-380) in an extended conformation. The binding of bestatin is quite different as was found in the complex between bestatin and bovine lens leucine amino-peptidase (bLLAP) (Burley, S., David, P., Sweet, R., Taylor, A. & Lipscomb, W. *J. Mol. Biol.* **224**, 113-140 (1992)). In that complex, bestatin was bound to the Zn by both the terminal nitrogen and the nonproteinaceous P1 hydroxyl oxygen, while in LTA<sub>4</sub> hydrolase the bestatin is bound by the hydroxyl and carbonyl oxygens. The terminal nitrogen is involved in hydrogen bonding to Glu271 and Gln136. These differences



could stem from the fact the bLAP is a bimetal protein with a different reaction mechanism. Moreover the binding of bestatin as seen in LTA4 hydrolase is similar with the complexes formed between thermolysin and hydroxamates which also act as bidentate ligands by the hydroxyl and carbonyl oxygens (Holmes, M. & Matthews, B. *Biochemistry* 20 (1981)).

Behind the pocket in which the phenyl ring of bestatin binds, there is a cavity that stretches 15 Å deeper into the protein and is approximately 6 to 7 Å wide. In the present structure this cavity is filled with water molecules. It has however a very hydrophobic nature and is lined with Trp311, Phe314, Trp315 Phe362, Leu365, Val367, Leu369, Pro374, Ala377, Tyr378, and Pro382. Most of these residues are strictly conserved or conserved in nature in all LTA4 hydrolase sequences known up until now, with the exception of Val367, which is replaced by a Gln in the yeast and *C. elegans* sequences. Interestingly space for this cavity is partly created by the interruption by the extended conformation in the stretch where Tyr378 and Tyr383 are found. One patch of this binding site is quite hydrophilic with Asn134, Asp375 and the OH of Tyr267 clustering together. This bigger cavity could be a binding site for the LTA4 substrate molecule. If the epoxide moiety would bind in a similar way as the carbonyl oxygen of bestatin to the Zn ion, then the hydrophobic tail would fit snugly into the binding site now occupied by the phenyl group of bestatin and would continue into the deeper hydrophobic cavity (Fig. 9a). The other tail would sit in the pocket that is now occupied by the carboxy group of bestatin and it would be long enough for the carboxylic acid to make direct electrostatic interactions with the conserved Arg563 and Lys565.

The replacement of Val367 by Gln as seen in the enzyme from yeast would make the hydrophobic channel shorter and this might be one of the reasons why the yeast enzyme does not have leukotriene A4 epoxide hydrolase activity. The manner in which the leukotriene molecule would bind is similar as what is proposed for binding of arachidonic acid in 15-lipoxygenase (Gillmor, S.A., Villasenor, A.,



Fletterick, R., Sigal, E. & Browner, M.F. *Nature Struc. Biol.* 4, 1003-1009 (1997)) with the hydrophobic end buried inside the protein and the carboxylic acid more towards the surface making interactions with Arg and Lys residues.

The binding of bestatin acts also as a guide for the binding of peptide substrate molecules. From systematic binding studies with tri-peptides it was shown that the enzyme has a strong preference for an arginine residue as the N-terminal residue and for several tri-peptides the enzyme has a  $k_{cat}/K_m$  ratio 10-fold the  $k_{cat}/K_m$  for LTA4 (Örning, L., Gierse, J.K. & Fitzpatrick, F.A. *J. Biol. Chem.* 269, 11269-11273 (1994). If we roughly model a peptide in the active site with an N-terminal Arg with the carbonyl oxygen sitting on the place of the hydroxyl group of bestatin, then the Arg side-chain of this residue would sit in the same place as the phenyl group of the bestatin with the guanidinium headgroup interacting with the conserved Asp375 and the OH of Tyr267 and the more hydrophobic C $\beta$ , C $\delta$  and C $\epsilon$  atoms making similar interactions as the phenyl ring. The terminal aminogroup could make the same electrostatic interaction as the terminal aminogroup of bestatin with Asp271 and Gln136. This mode of binding of bestatin is in contrast with the mode proposed by Örning, since the phenyl ring seems to occupy the S1 pocket. We also propose that the LTA4 substrate molecule is occupying all three pockets, S1, S'1 and S'2.

If the binding mode of peptides in LTA4 hydrolase is compared with the one described for thermolysin, a number of differences are observed. In thermolysin, the peptide molecule is held in place by many interactions to the main chain atoms provided by Asn112, Ala203, Arg203 and Trp115. None of these residues or equivalent residues can be found in the binding site in LTA4 hydrolase. Furthermore, although binding pockets S1 and S'1 are at similar positions as in thermolysin, site S'2 has to be different since its space is occupied by Tyr378 in LTA4 hydrolase. Glu271 and Gln136 and the N-terminal domain are filling up the space into which in thermolysin the upstream peptide binds contributing to the exopeptidase function instead of an endo-peptidase function as in thermolysin.



#### 4.6 Putative Phosphorylation site

Recently specific phosphorylation by a yet unknown specific kinase of Ser415 has been described as means of regulation of LTA4 hydrolase activity in endothelial cells (Rybina, I.V., Liu, H., Gor, Y. & Feinmark, S.J. *J Biol Chem* **272**, 31865-71 (1997)). This residue is conserved in all mammalian LTA4 hydrolases and is embedded in a highly homologous stretch of residues. Phosphorylation of this residue seems to inhibit the epoxide hydrolase activity but not the amino-peptidase activity. In the structure this residue is located in a loop connecting two  $\alpha$ -helices that lie on the surface of the molecule. The loop itself is located at the back of the enzyme.

#### 4.7 Aminopeptidase activity

The amino-peptidase activity catalyzed by this enzyme has been well studied and many of the important residues have been target for site-directed mutagenesis work. This lead to a proposal in which Glu296 would act as a general base (Wetterholm, A., *et al. Proc Natl Acad Sci U S A* **89**, 9141-9145 (1992)) and Tyr383 as a putative proton donor (Blomster, M., Wetterholm, A., Mueller, M.J. & Haeggström, J.Z. *Eur. J. Biochem.* **231**, 528-534 (1995)). In the current complex, these residues are involved in hydrogen bonds with the bestatin molecule. If bestatin binding is seen as a rough analog for the transition state binding, then the interaction of Glu296 with the hydroxyl oxygen of bestatin indicates that this residue could indeed activate a water-molecule for the nucleophilic attack. The role of Tyr383 cannot so easily be confirmed, however its position strongly suggest the role of proton donor. In ther-



molysin the proton donor is His231 and although the Ca position of this residue is 4.1Å removed from the Ca position of Tyr383 in LTA4 hydrolase, the Nd1 is only 1 Å removed from the OH position of Tyr383. The conserved Glu271 could be involved in the exo-protease activity of the protein. Recently, the analogous Glu350 in aminopeptidase N and Glu352 in aminopeptidase A were subject to site-directed mutagenesis work (Luciani, N., *et al. Biochemistry* **37**, 686-692 (1998); and Vazeux, G., Iturrioz, X., Corvol, P. & Llorenz-Cortez, C. *Biochem. J.* **334**, 407-413 (1998)) and it was observed that mutations of this residue lead to large decreases in the activity in the case of substitutions by conserved amino-acids such as aspartate and glutamine and absence of activity in substitution by alanine. It was concluded that Glu350 belonged to the anionic binding site in that protein. A mechanism based on thermolysin was proposed for aminopeptidase N with a pentavalent transition state with an additional interaction between the free  $\alpha$ -aminogroup and Glu350. In this structure we can observe such an interaction between Glu271 and the free aminogroup of bestatin. Furthermore the penta-valent coordination of Zn by the His295, His299, Glu318 and the carbonyl and hydroxyl groups of bestatin indicates that this is an equivalent transition state analog complex as determined previously for thermolysin.

From careful sequence alignments and structural insight we can conclude that the enzymes in the M1 family of proteases will share a highly conserved catalytic domain that includes part of the N-terminal domain as we see it in LTA4 hydrolase and the thermolysin-like domain. There is no homology for residues in the C-terminal domain and we believe that this domain is unique for LTA4 hydrolases. We suggest that all proteases belonging to class M1 with the signature HExxH and a Glu 18 residues downstream will function in a similar way to thermolysin.

#### 4.8 Epoxide hydrolase activity



Concerning the epoxide hydrolase activity, much less is known about the functional elements and mechanisms of catalysis. In fact, the prosthetic zinc is the only critical component identified thus far and may potentially assist in the introduction of a water molecule at C12 or in the activation of the epoxide. Although Tyr378 and Tyr383 are important active side residues, none of them is essential for catalysis. A mutation of Tyr378 to Phe protects the enzyme against suicide inhibition, however the specificity of the double bond configuration is partly lost (Mueller, M., Andberg, M., Samuelsson, B. & Haeggstrom, J. *J. Biol. Chem.* **271**, 24345-24348 (1996)) since a novel metabolite with a *cis-trans-cis* conjugated system can be detected. Thus, Tyr378 is a major binding site for LTA<sub>4</sub> during suicide inactivation and seems to play a role for the formation of the correct double bond geometry in the product LTB<sub>4</sub>. Mutations of Tyr383 abolish the amino-peptidase activity where it has a role as potential proton donor (*vide supra*) but the epoxide hydrolase activity is only decreased compared to wild-type. It is however implicated in the stereospecific introduction of water during the hydrolysis of LTA<sub>4</sub> to LTB<sub>4</sub> since these mutants convert LTA<sub>4</sub> in both LTB<sub>4</sub> and 5 [S],6 [S]-DHETE (Andberg, M., Hamberg, M. & Haeggstrom, J. *J. Biol. Chem.* **272**, 23057-23063 (1997)). Moreover careful analysis of the catalytic properties of enzymes mutated in pos. 383, *viz* [Y383F], [Y383H] and [Y383Q]LTA<sub>4</sub> hydrolase have indicated that the epoxide hydrolase reaction follows an SN1 mechanism.

If one considers the chemistry carried out by LTA<sub>4</sub> hydrolase, the enzyme has two major tasks during the hydrolysis of LTA<sub>4</sub> to LTB<sub>4</sub>. First introduction of a water molecule stereospecific at C12 and second to generate a *cis*-double bond  $\Delta^6$  in the resulting conjugated triene system [cf. Fig. 1]. If LTA<sub>4</sub> is modeled into the putative substrate binding pocket as indicated in figure 9b, the catalytic zinc gets close to the epoxide and not C12 of the substrate. Therefore the most likely role of the Zn ion is to act directly as a Lewis acid to activate and open the epoxide ring. This would generate a carbocation, whose charge will be delocalised over the



conjugated triene system from C7 to C12. Since this intermediate has an *sp*<sup>2</sup> hybridized planar configuration at C12, it is in principle open for nucleophilic attack from either side of the molecule. The conserved Asp375 is positioned in such a way that a water molecule bound to it is in “attacking” distance of C12 of a modeled LTA<sub>4</sub> molecule, the position into which a hydroxyl group is inserted during the reaction. This will account for the proper stereo-chemical and positional insertion of the hydroxyl-group at C12 in *R* configuration.

The shape and curvature of the LTA<sub>4</sub> binding pocket also gives a clue as to how the enzyme creates the *cis* double bond at  $\Delta$ 6. Since there is free rotation between the c6 and c7 of LTA<sub>4</sub>, this bond may be kept in a “pro-*cis*” configuration in the transition state, which in turn would facilitate the formation of a  $\Delta$ 6-*cis* double bond from the carbocation intermediate. If LTA<sub>4</sub> is modeled in this way, the entire molecule adopts a bent shape, fitting very well with the architecture of the binding pocket (Fig. 9b). Hence, the critical double bond geometry at  $\Delta$ 6 of LTB<sub>4</sub> is probably guaranteed by the exact binding conformation of LTA<sub>4</sub> at the active side which in turn is governed by all the structural elements participating in substrate binding, including the carboxylate recognition sites, Arg56 and Lys565, the catalytic zinc and the hydrophobic residues lining the pocket. The putative binding cleft for the leukotriene molecule is narrow and bent and thereby favoring LTA<sub>4</sub> over other epoxides. The two tyrosines are positioned such that they are in contact with the triple double bond configuration of a modeled LTA<sub>4</sub> molecule at the bent of the putative binding pocket and they are hydrogen-bonded to each other. Therefore their position is ideal for guidance in stereo-specificity of the double bond configuration. The loss of specificity for the hydroxyl-incorporation at the C12 position in case of the Tyr383 position can be explained that mutations at this position would possibly create extra space for a water molecule that could attack at the C6 position and thereby form 5 [S],6 [S]-DHETE.



The position of Tyr378 is such that it is in contact with the C6 atom of the modeled LTA4 molecule. If after opening of the epoxide ring the hydroxyl group of Tyr378 instead of a water molecule would attack the carbon-cation at the C6 position, a covalently attached molecule is formed which forms the suicide inhibited complex. In order to check this hypothesis and to obtain more information about the binding-site for leukotriene A4, the structure of this inhibited species would be essential.

In order to exclude the possibility that residues near the active site might have further catalytic roles in the epoxide hydrolase reaction, a thorough investigation of these residues, such as Glu271 and Gln136 has to be started. Furthermore the proposed role of Asp375 in activating a water molecule for the stereospecific attack at C12 has to be investigated.

Accordingly, the present invention has solved the first specific leukotriene converting enzyme, which for the first time reveals the binding mode for leukotriene molecules. Furthermore, insight is provided in a unique active site that harbours two activities using different amino-acids to catalyze different reactions.



## 5. SEQUENCE LISTING

<110> Haeggström, Jesper J.Z., et al

<120> DRUG DESIGN BASED ON THE STRUCTURE OF LTA<sub>4</sub> HYDROLASE

<130> 54660

<140>

<141>

<160> 1

<170> PatentIn Ver. 2.1

<210> 1

<211> 611

<212> PRT

<213> HUMAN

<220>

<223> AMINO ACID SEQUENCE OF HUMAN LEUKOTRIENE A<sub>4</sub>  
HYDROLASE

<400> 1

Met Pro Glu Ile Val Asp Thr Cys Ser Leu Ala Ser Pro Ala Ser Val  
1 5 10 15

Cys Arg Thr Lys His Leu His Leu Arg Cys Ser Val Asp Phe Thr Arg  
20 25 30

Arg Thr Leu Thr Gly Thr Ala Ala Leu Thr Val Gln Ser Gln Glu Asp  
35 40 45

Asn Leu Arg Ser Leu Val Leu Asp Thr Lys Asp Leu Thr Ile Glu Lys  
50 55 60

Val Val Ile Asn Gly Gln Glu Val Lys Tyr Ala Leu Gly Glu Arg Gln  
65 70 75 80

Ser Tyr Lys Gly Ser Pro Met Glu Ile Ser Leu Pro Ile Ala Leu Ser  
85 90 95



Lys Asn Gln Glu Ile Val Ile Glu Ile Ser Phe Glu Thr Ser Pro Lys  
100 105 110

Ser Ser Ala Leu Gln Trp Leu Thr Pro Glu Gln Thr Ser Gly Lys Glu  
115 120 125

His Pro Tyr Leu Phe Ser Gln Cys Gln Ala Ile His Cys Arg Ala Ile  
130 135 140

Leu Pro Cys Gln Asp Thr Pro Ser Val Lys Leu Thr Tyr Thr Ala Glu  
145 150 155 160

Val Ser Val Pro Lys Glu Leu Val Ala Leu Met Ser Ala Ile Arg Asp  
165 170 175

Gly Glu Thr Pro Asp Pro Glu Asp Pro Ser Arg Lys Ile Tyr Lys Phe  
180 185 190

Ile Gln Lys Val Pro Ile Pro Cys Tyr Leu Ile Ala Leu Val Val Gly  
195 200 205

Ala Leu Glu Ser Arg Gln Ile Gly Pro Arg Thr Leu Val Trp Ser Glu  
210 215 220

Lys Glu Gln Val Glu Lys Ser Ala Tyr Glu Phe Ser Glu Thr Glu Ser  
225 230 235 240

Met Leu Lys Ile Ala Glu Asp Leu Gly Gly Pro Tyr Val Trp Gly Gln  
245 250 255

Tyr Asp Leu Leu Val Leu Pro Pro Ser Phe Pro Tyr Gly Gly Met Glu  
260 265 270

Asn Pro Cys Leu Thr Phe Val Thr Pro Thr Leu Leu Ala Gly Asp Lys  
275 280 285

Ser Leu Ser Asn Val Ile Ala His Glu Ile Ser His Ser Trp Thr Gly  
290 295 300

Asn Leu Val Thr Asn Lys Thr Trp Asp His Phe Trp Leu Asn Glu Gly  
305 310 315 320

His Thr Val Tyr Leu Glu Arg His Ile Cys Gly Arg Leu Phe Gly Glu



|   |     |     |
|---|-----|-----|
| 325   | 330 | 335 |
| Lys Phe Arg His Phe Asn Ala Leu Gly Gly Trp Gly Glu Leu Gln Asn |     |     |
| 340   | 345 | 350 |
| Ser Val Lys Thr Phe Gly Glu Thr His Pro Phe Thr Lys Leu Val Val |     |     |
| 355   | 360 | 365 |
| Asp Leu Thr Asp Ile Asp Pro Asp Val Ala Tyr Ser Ser Val Pro Tyr |     |     |
| 370   | 375 | 380 |
| Glu Lys Gly Phe Ala Leu Leu Phe Tyr Leu Glu Gln Leu Leu Gly Gly |     |     |
| 385   | 390 | 395 |
| Pro Glu Ile Phe Leu Gly Phe Leu Lys Ala Tyr Val Glu Lys Phe Ser |     |     |
| 405   | 410 | 415 |
| Tyr Lys Ser Ile Thr Thr Asp Asp Trp Lys Asp Phe Leu Tyr Ser Tyr |     |     |
| 420   | 425 | 430 |
| Phe Lys Asp Lys Val Asp Val Leu Asn Gln Val Asp Trp Asn Ala Trp |     |     |
| 435   | 440 | 445 |
| Leu Tyr Ser Pro Gly Leu Pro Pro Ile Lys Pro Asn Tyr Asp Met Thr |     |     |
| 450   | 455 | 460 |
| Leu Thr Asn Ala Cys Ile Ala Leu Ser Gln Arg Trp Ile Thr Ala Lys |     |     |
| 465   | 470 | 475 |
| Glu Asp Asp Leu Asn Ser Phe Asn Ala Thr Asp Leu Lys Asp Leu Ser |     |     |
| 485   | 490 | 495 |
| Ser His Gln Leu Asn Glu Phe Leu Ala Gln Thr Leu Gln Arg Ala Pro |     |     |
| 500   | 505 | 510 |
| Leu Pro Leu Gly His Ile Lys Arg Met Gln Glu Val Tyr Asn Phe Asn |     |     |
| 515   | 520 | 525 |
| Ala Ile Asn Asn Ser Glu Ile Arg Phe Arg Trp Leu Arg Leu Cys Ile |     |     |
| 530   | 535 | 540 |
| Gln Ser Lys Trp Glu Asp Ala Ile Pro Leu Ala Leu Lys Met Ala Thr |     |     |
| 545   | 550 | 555 |
|   |     | 560 |



Glu Gln Gly Arg Met Lys Phe Thr Arg Pro Leu Phe Lys Asp Leu Ala  
565 570 575

Ala Phe Asp Lys Ser His Asp Gln Ala Val Arg Thr Tyr Gln Glu His  
580 585 590

Lys Ala Ser Met His Pro Val Thr Ala Met Leu Val Gly Lys Asp Leu  
595 600 605

Lys Val Asp  
610

009220 DT 22709



## 6. CONFORMATIONAL DATA

Table 9: Structure coordinates of LTA<sub>4</sub> hydrolase-bestatin complex

|        |          |          |          |       |       |          |
|--------|----------|----------|----------|-------|-------|----------|
| CRYST1 | 67.585   | 133.510  | 83.400   | 90.00 | 90.00 | 90.00    |
| ORIGX1 | 1.000000 | 0.000000 | 0.000000 |       |       | 0.000000 |
| ORIGX2 | 0.000000 | 1.000000 | 0.000000 |       |       | 0.000000 |
| ORIGX3 | 0.000000 | 0.000000 | 1.000000 |       |       | 0.000000 |
| SCALE1 | 0.014796 | 0.000000 | 0.000000 |       |       | 0.000000 |
| SCALE2 | 0.000000 | 0.007490 | 0.000000 |       |       | 0.000000 |
| SCALE3 | 0.000000 | 0.000000 | 0.011990 |       |       | 0.000000 |

|      | Atom | res. | Chain No. | x      | y      | z      | occ  | B-factor |
|------|------|------|-----------|--------|--------|--------|------|----------|
| ATOM | 1    | N    | PRO A 1   | -2.496 | 16.950 | 65.263 | 1.00 | 100.00   |
| ATOM | 2    | CA   | PRO A 1   | -1.236 | 17.634 | 65.508 | 1.00 | 99.43    |
| ATOM | 3    | C    | PRO A 1   | -1.279 | 19.127 | 65.159 | 1.00 | 99.95    |
| ATOM | 4    | O    | PRO A 1   | -0.289 | 19.676 | 64.664 | 1.00 | 100.00   |
| ATOM | 5    | CB   | PRO A 1   | -0.177 | 16.885 | 64.670 | 1.00 | 100.00   |
| ATOM | 6    | CG   | PRO A 1   | -0.850 | 15.680 | 64.020 | 1.00 | 100.00   |
| ATOM | 7    | CD   | PRO A 1   | -2.318 | 15.723 | 64.426 | 1.00 | 99.22    |
| ATOM | 8    | N    | GLU A 2   | -2.412 | 19.789 | 65.446 | 1.00 | 90.69    |
| ATOM | 9    | CA   | GLU A 2   | -2.616 | 21.205 | 65.132 | 1.00 | 88.44    |
| ATOM | 10   | C    | GLU A 2   | -1.945 | 22.313 | 65.960 | 1.00 | 86.73    |
| ATOM | 11   | O    | GLU A 2   | -2.129 | 22.438 | 67.174 | 1.00 | 88.87    |
| ATOM | 12   | CB   | GLU A 2   | -4.088 | 21.530 | 64.831 | 1.00 | 89.80    |
| ATOM | 13   | CG   | GLU A 2   | -4.228 | 22.312 | 63.514 | 1.00 | 95.02    |
| ATOM | 14   | CD   | GLU A 2   | -3.125 | 21.962 | 62.559 | 1.00 | 100.00   |
| ATOM | 15   | OE1  | GLU A 2   | -2.011 | 22.486 | 62.601 | 1.00 | 70.64    |
| ATOM | 16   | OE2  | GLU A 2   | -3.487 | 21.008 | 61.722 | 1.00 | 83.56    |
| ATOM | 17   | N    | ILE A 3   | -1.177 | 23.171 | 65.274 | 1.00 | 73.36    |
| ATOM | 18   | CA   | ILE A 3   | -0.495 | 24.292 | 65.914 | 1.00 | 69.05    |
| ATOM | 19   | C    | ILE A 3   | -1.215 | 25.619 | 65.639 | 1.00 | 60.01    |
| ATOM | 20   | O    | ILE A 3   | -1.489 | 25.975 | 64.480 | 1.00 | 56.74    |
| ATOM | 21   | CB   | ILE A 3   | 1.014  | 24.323 | 65.649 | 1.00 | 73.58    |
| ATOM | 22   | CG1  | ILE A 3   | 1.560  | 25.747 | 65.693 | 1.00 | 73.27    |
| ATOM | 23   | CG2  | ILE A 3   | 1.360  | 23.656 | 64.319 | 1.00 | 79.61    |
| ATOM | 24   | CD1  | ILE A 3   | 3.062  | 25.814 | 65.946 | 1.00 | 75.66    |
| ATOM | 25   | N    | VAL A 4   | -1.530 | 26.333 | 66.734 | 1.00 | 46.96    |
| ATOM | 26   | CA   | VAL A 4   | -2.266 | 27.598 | 66.688 | 1.00 | 41.58    |
| ATOM | 27   | C    | VAL A 4   | -1.472 | 28.880 | 66.873 | 1.00 | 30.92    |
| ATOM | 28   | O    | VAL A 4   | -0.723 | 29.061 | 67.838 | 1.00 | 28.33    |
| ATOM | 29   | CB   | VAL A 4   | -3.441 | 27.614 | 67.680 | 1.00 | 45.38    |
| ATOM | 30   | CG1  | VAL A 4   | -4.362 | 28.831 | 67.511 | 1.00 | 44.59    |
| ATOM | 31   | CG2  | VAL A 4   | -4.271 | 26.359 | 67.495 | 1.00 | 45.63    |
| ATOM | 32   | N    | ASP A 5   | -1.727 | 29.798 | 65.947 | 1.00 | 22.16    |
| ATOM | 33   | CA   | ASP A 5   | -1.139 | 31.105 | 66.027 | 1.00 | 21.88    |
| ATOM | 34   | C    | ASP A 5   | -2.103 | 31.939 | 66.842 | 1.00 | 25.15    |
| ATOM | 35   | O    | ASP A 5   | -3.064 | 32.490 | 66.346 | 1.00 | 21.09    |
| ATOM | 36   | CB   | ASP A 5   | -0.915 | 31.761 | 64.661 | 1.00 | 21.53    |
| ATOM | 37   | CG   | ASP A 5   | -0.170 | 33.040 | 64.836 | 1.00 | 21.15    |
| ATOM | 38   | OD1  | ASP A 5   | -0.200 | 33.672 | 65.879 | 1.00 | 23.73    |
| ATOM | 39   | OD2  | ASP A 5   | 0.484  | 33.404 | 63.754 | 1.00 | 18.74    |
| ATOM | 40   | N    | THR A 6   | -1.812 | 32.004 | 68.122 | 1.00 | 22.87    |
| ATOM | 41   | CA   | THR A 6   | -2.614 | 32.733 | 69.039 | 1.00 | 17.86    |
| ATOM | 42   | C    | THR A 6   | -2.468 | 34.218 | 68.837 | 1.00 | 25.17    |
| ATOM | 43   | O    | THR A 6   | -3.013 | 35.005 | 69.583 | 1.00 | 32.74    |
| ATOM | 44   | CB   | THR A 6   | -2.366 | 32.263 | 70.467 | 1.00 | 28.19    |



|      |     |     |     |   |    |         |        |        |      |       |
|------|-----|-----|-----|---|----|---------|--------|--------|------|-------|
| ATOM | 45  | OG1 | THR | A | 6  | -0.986  | 32.305 | 70.759 | 1.00 | 31.35 |
| ATOM | 46  | CG2 | THR | A | 6  | -2.827  | 30.824 | 70.556 | 1.00 | 24.61 |
| ATOM | 47  | N   | CYS | A | 7  | -1.756  | 34.657 | 67.824 | 1.00 | 19.01 |
| ATOM | 48  | CA  | CYS | A | 7  | -1.687  | 36.105 | 67.594 | 1.00 | 18.86 |
| ATOM | 49  | C   | CYS | A | 7  | -2.514  | 36.534 | 66.364 | 1.00 | 27.36 |
| ATOM | 50  | O   | CYS | A | 7  | -2.589  | 37.717 | 66.031 | 1.00 | 24.81 |
| ATOM | 51  | CB  | CYS | A | 7  | -0.244  | 36.638 | 67.389 | 1.00 | 19.56 |
| ATOM | 52  | SG  | CYS | A | 7  | 0.817   | 36.357 | 68.834 | 1.00 | 23.65 |
| ATOM | 53  | N   | SER | A | 8  | -3.077  | 35.572 | 65.619 | 1.00 | 28.38 |
| ATOM | 54  | CA  | SER | A | 8  | -3.820  | 35.920 | 64.408 | 1.00 | 25.64 |
| ATOM | 55  | C   | SER | A | 8  | -5.279  | 35.549 | 64.559 | 1.00 | 25.67 |
| ATOM | 56  | O   | SER | A | 8  | -5.622  | 34.573 | 65.244 | 1.00 | 20.89 |
| ATOM | 57  | CB  | SER | A | 8  | -3.286  | 35.203 | 63.175 | 1.00 | 27.58 |
| ATOM | 58  | OG  | SER | A | 8  | -4.110  | 35.477 | 62.050 | 1.00 | 26.21 |
| ATOM | 59  | N   | LEU | A | 9  | -6.127  | 36.354 | 63.928 | 1.00 | 23.57 |
| ATOM | 60  | CA  | LEU | A | 9  | -7.555  | 36.054 | 64.006 | 1.00 | 24.90 |
| ATOM | 61  | C   | LEU | A | 9  | -8.006  | 35.381 | 62.706 | 1.00 | 26.66 |
| ATOM | 62  | O   | LEU | A | 9  | -9.114  | 34.912 | 62.612 | 1.00 | 28.44 |
| ATOM | 63  | CB  | LEU | A | 9  | -8.411  | 37.332 | 64.224 | 1.00 | 22.92 |
| ATOM | 64  | CG  | LEU | A | 9  | -8.092  | 38.121 | 65.494 | 1.00 | 24.11 |
| ATOM | 65  | CD1 | LEU | A | 9  | -8.997  | 39.353 | 65.644 | 1.00 | 25.94 |
| ATOM | 66  | CD2 | LEU | A | 9  | -8.302  | 37.203 | 66.698 | 1.00 | 16.04 |
| ATOM | 67  | N   | ALA | A | 10 | -7.137  | 35.392 | 61.699 | 1.00 | 23.67 |
| ATOM | 68  | CA  | ALA | A | 10 | -7.378  | 34.838 | 60.373 | 1.00 | 20.08 |
| ATOM | 69  | C   | ALA | A | 10 | -7.559  | 33.342 | 60.324 | 1.00 | 23.49 |
| ATOM | 70  | O   | ALA | A | 10 | -7.321  | 32.597 | 61.261 | 1.00 | 22.41 |
| ATOM | 71  | CB  | ALA | A | 10 | -6.365  | 35.297 | 59.334 | 1.00 | 18.72 |
| ATOM | 72  | N   | SER | A | 11 | -8.066  | 32.886 | 59.190 | 1.00 | 26.45 |
| ATOM | 73  | CA  | SER | A | 11 | -8.239  | 31.460 | 59.014 | 1.00 | 27.04 |
| ATOM | 74  | C   | SER | A | 11 | -6.821  | 30.862 | 58.977 | 1.00 | 19.63 |
| ATOM | 75  | O   | SER | A | 11 | -5.931  | 31.368 | 58.288 | 1.00 | 20.98 |
| ATOM | 76  | CB  | SER | A | 11 | -8.972  | 31.228 | 57.683 | 1.00 | 34.23 |
| ATOM | 77  | OG  | SER | A | 11 | -10.377 | 31.332 | 57.861 | 1.00 | 36.98 |
| ATOM | 78  | N   | PRO | A | 12 | -6.609  | 29.777 | 59.689 | 1.00 | 20.69 |
| ATOM | 79  | CA  | PRO | A | 12 | -5.293  | 29.146 | 59.759 | 1.00 | 23.75 |
| ATOM | 80  | C   | PRO | A | 12 | -4.838  | 28.466 | 58.479 | 1.00 | 32.70 |
| ATOM | 81  | O   | PRO | A | 12 | -5.628  | 28.213 | 57.566 | 1.00 | 34.79 |
| ATOM | 82  | CB  | PRO | A | 12 | -5.378  | 28.124 | 60.898 | 1.00 | 24.49 |
| ATOM | 83  | CG  | PRO | A | 12 | -6.850  | 27.923 | 61.197 | 1.00 | 26.79 |
| ATOM | 84  | CD  | PRO | A | 12 | -7.620  | 28.984 | 60.422 | 1.00 | 18.71 |
| ATOM | 85  | N   | ALA | A | 13 | -3.542  | 28.158 | 58.424 | 1.00 | 28.05 |
| ATOM | 86  | CA  | ALA | A | 13 | -2.958  | 27.522 | 57.254 | 1.00 | 26.23 |
| ATOM | 87  | C   | ALA | A | 13 | -3.575  | 26.147 | 56.955 | 1.00 | 22.95 |
| ATOM | 88  | O   | ALA | A | 13 | -3.463  | 25.623 | 55.868 | 1.00 | 25.46 |
| ATOM | 89  | CB  | ALA | A | 13 | -1.432  | 27.511 | 57.312 | 1.00 | 24.61 |
| ATOM | 90  | N   | SER | A | 14 | -4.227  | 25.555 | 57.935 | 1.00 | 21.79 |
| ATOM | 91  | CA  | SER | A | 14 | -4.840  | 24.254 | 57.758 | 1.00 | 23.68 |
| ATOM | 92  | C   | SER | A | 14 | -6.239  | 24.371 | 57.129 | 1.00 | 32.59 |
| ATOM | 93  | O   | SER | A | 14 | -6.977  | 23.401 | 56.944 | 1.00 | 34.73 |
| ATOM | 94  | CB  | SER | A | 14 | -4.921  | 23.533 | 59.102 | 1.00 | 26.34 |
| ATOM | 95  | OG  | SER | A | 14 | -5.722  | 24.269 | 60.022 | 1.00 | 28.63 |
| ATOM | 96  | N   | VAL | A | 15 | -6.632  | 25.589 | 56.814 | 1.00 | 28.74 |
| ATOM | 97  | CA  | VAL | A | 15 | -7.913  | 25.838 | 56.183 | 1.00 | 29.68 |
| ATOM | 98  | C   | VAL | A | 15 | -7.714  | 26.415 | 54.790 | 1.00 | 28.85 |
| ATOM | 99  | O   | VAL | A | 15 | -8.284  | 25.983 | 53.793 | 1.00 | 30.55 |
| ATOM | 100 | CB  | VAL | A | 15 | -8.736  | 26.750 | 57.064 | 1.00 | 33.16 |
| ATOM | 101 | CG1 | VAL | A | 15 | -9.867  | 27.390 | 56.256 | 1.00 | 32.75 |
| ATOM | 102 | CG2 | VAL | A | 15 | -9.232  | 25.957 | 58.267 | 1.00 | 30.08 |



|      |     |     |     |   |    |        |        |        |      |        |
|------|-----|-----|-----|---|----|--------|--------|--------|------|--------|
| ATOM | 103 | N   | CYS | A | 16 | -6.856 | 27.406 | 54.714 | 1.00 | 22.64  |
| ATOM | 104 | CA  | CYS | A | 16 | -6.559 | 28.009 | 53.440 | 1.00 | 25.21  |
| ATOM | 105 | C   | CYS | A | 16 | -5.237 | 28.693 | 53.559 | 1.00 | 29.42  |
| ATOM | 106 | O   | CYS | A | 16 | -4.779 | 28.929 | 54.690 | 1.00 | 29.35  |
| ATOM | 107 | CB  | CYS | A | 16 | -7.621 | 28.958 | 52.872 | 1.00 | 29.68  |
| ATOM | 108 | SG  | CYS | A | 16 | -7.936 | 30.421 | 53.895 | 1.00 | 35.74  |
| ATOM | 109 | N   | ARG | A | 17 | -4.637 | 28.959 | 52.405 | 1.00 | 23.28  |
| ATOM | 110 | CA  | ARG | A | 17 | -3.332 | 29.581 | 52.397 | 1.00 | 27.42  |
| ATOM | 111 | C   | ARG | A | 17 | -3.224 | 30.603 | 51.288 | 1.00 | 29.92  |
| ATOM | 112 | O   | ARG | A | 17 | -3.516 | 30.317 | 50.133 | 1.00 | 30.00  |
| ATOM | 113 | CB  | ARG | A | 17 | -2.205 | 28.555 | 52.227 | 1.00 | 23.72  |
| ATOM | 114 | CG  | ARG | A | 17 | -2.233 | 27.401 | 53.201 | 1.00 | 21.97  |
| ATOM | 115 | CD  | ARG | A | 17 | -1.407 | 26.256 | 52.647 | 1.00 | 23.54  |
| ATOM | 116 | NE  | ARG | A | 17 | -0.812 | 25.328 | 53.619 | 1.00 | 61.25  |
| ATOM | 117 | CZ  | ARG | A | 17 | -1.432 | 24.397 | 54.351 | 1.00 | 74.57  |
| ATOM | 118 | NH1 | ARG | A | 17 | -2.727 | 24.196 | 54.302 | 1.00 | 81.15  |
| ATOM | 119 | NH2 | ARG | A | 17 | -0.734 | 23.629 | 55.172 | 1.00 | 66.19  |
| ATOM | 120 | N   | THR | A | 18 | -2.752 | 31.787 | 51.640 | 1.00 | 19.72  |
| ATOM | 121 | CA  | THR | A | 18 | -2.591 | 32.805 | 50.644 | 1.00 | 16.81  |
| ATOM | 122 | C   | THR | A | 18 | -1.334 | 32.493 | 49.887 | 1.00 | 26.15  |
| ATOM | 123 | O   | THR | A | 18 | -0.323 | 32.299 | 50.512 | 1.00 | 28.80  |
| ATOM | 124 | CB  | THR | A | 18 | -2.466 | 34.204 | 51.296 | 1.00 | 25.57  |
| ATOM | 125 | OG1 | THR | A | 18 | -3.626 | 34.537 | 52.038 | 1.00 | 29.71  |
| ATOM | 126 | CG2 | THR | A | 18 | -2.186 | 35.291 | 50.261 | 1.00 | 23.47  |
| ATOM | 127 | N   | LYS | A | 19 | -1.361 | 32.518 | 48.568 | 1.00 | 23.41  |
| ATOM | 128 | CA  | LYS | A | 19 | -0.185 | 32.210 | 47.806 | 1.00 | 21.13  |
| ATOM | 129 | C   | LYS | A | 19 | 0.459  | 33.389 | 47.154 | 1.00 | 22.88  |
| ATOM | 130 | O   | LYS | A | 19 | 1.643  | 33.365 | 46.806 | 1.00 | 26.65  |
| ATOM | 131 | CB  | LYS | A | 19 | -0.542 | 31.198 | 46.727 | 1.00 | 29.31  |
| ATOM | 132 | CG  | LYS | A | 19 | -1.357 | 30.002 | 47.207 | 1.00 | 38.67  |
| ATOM | 133 | CD  | LYS | A | 19 | -0.856 | 29.376 | 48.505 | 1.00 | 83.39  |
| ATOM | 134 | CE  | LYS | A | 19 | 0.228  | 28.313 | 48.317 | 1.00 | 100.00 |
| ATOM | 135 | NZ  | LYS | A | 19 | 0.082  | 27.127 | 49.186 | 1.00 | 95.09  |
| ATOM | 136 | N   | HIS | A | 20 | -0.334 | 34.419 | 46.949 | 1.00 | 19.69  |
| ATOM | 137 | CA  | HIS | A | 20 | 0.217  | 35.576 | 46.285 | 1.00 | 19.81  |
| ATOM | 138 | C   | HIS | A | 20 | -0.586 | 36.810 | 46.644 | 1.00 | 28.29  |
| ATOM | 139 | O   | HIS | A | 20 | -1.767 | 36.712 | 47.018 | 1.00 | 30.86  |
| ATOM | 140 | CB  | HIS | A | 20 | 0.093  | 35.392 | 44.758 | 1.00 | 17.26  |
| ATOM | 141 | CG  | HIS | A | 20 | 0.795  | 36.466 | 44.024 | 1.00 | 19.73  |
| ATOM | 142 | ND1 | HIS | A | 20 | 2.171  | 36.455 | 43.885 | 1.00 | 22.73  |
| ATOM | 143 | CD2 | HIS | A | 20 | 0.305  | 37.600 | 43.437 | 1.00 | 20.99  |
| ATOM | 144 | CE1 | HIS | A | 20 | 2.491  | 37.554 | 43.201 | 1.00 | 21.23  |
| ATOM | 145 | NE2 | HIS | A | 20 | 1.386  | 38.269 | 42.903 | 1.00 | 20.99  |
| ATOM | 146 | N   | LEU | A | 21 | 0.073  | 37.954 | 46.508 | 1.00 | 25.18  |



|      |     |     |     |   |    |        |        |        |      |        |
|------|-----|-----|-----|---|----|--------|--------|--------|------|--------|
| ATOM | 161 | CD2 | HIS | A | 22 | 0.035  | 43.261 | 41.489 | 1.00 | 36.85  |
| ATOM | 162 | CE1 | HIS | A | 22 | -1.463 | 44.545 | 40.580 | 1.00 | 36.22  |
| ATOM | 163 | NE2 | HIS | A | 22 | -0.152 | 44.400 | 40.736 | 1.00 | 37.12  |
| ATOM | 164 | N   | LEU | A | 23 | -0.583 | 43.938 | 44.898 | 1.00 | 29.56  |
| ATOM | 165 | CA  | LEU | A | 23 | -0.842 | 45.192 | 45.558 | 1.00 | 30.11  |
| ATOM | 166 | C   | LEU | A | 23 | -0.590 | 46.398 | 44.661 | 1.00 | 32.22  |
| ATOM | 167 | O   | LEU | A | 23 | 0.486  | 46.685 | 44.121 | 1.00 | 32.37  |
| ATOM | 168 | CB  | LEU | A | 23 | -0.018 | 45.260 | 46.884 | 1.00 | 30.21  |
| ATOM | 169 | CG  | LEU | A | 23 | -0.410 | 46.274 | 47.982 | 1.00 | 33.02  |
| ATOM | 170 | CD1 | LEU | A | 23 | 0.663  | 47.343 | 48.117 | 1.00 | 32.82  |
| ATOM | 171 | CD2 | LEU | A | 23 | -1.745 | 46.956 | 47.745 | 1.00 | 38.23  |
| ATOM | 172 | N   | ARG | A | 24 | -1.656 | 47.133 | 44.534 | 1.00 | 34.49  |
| ATOM | 173 | CA  | ARG | A | 24 | -1.632 | 48.369 | 43.784 | 1.00 | 38.52  |
| ATOM | 174 | C   | ARG | A | 24 | -2.194 | 49.370 | 44.783 | 1.00 | 40.35  |
| ATOM | 175 | O   | ARG | A | 24 | -3.268 | 49.139 | 45.369 | 1.00 | 36.87  |
| ATOM | 176 | CB  | ARG | A | 24 | -2.487 | 48.307 | 42.521 | 1.00 | 45.90  |
| ATOM | 177 | CG  | ARG | A | 24 | -1.833 | 47.544 | 41.371 | 1.00 | 63.78  |
| ATOM | 178 | CD  | ARG | A | 24 | -2.551 | 47.750 | 40.046 | 1.00 | 88.27  |
| ATOM | 179 | NE  | ARG | A | 24 | -3.826 | 47.027 | 39.967 | 1.00 | 96.90  |
| ATOM | 180 | CZ  | ARG | A | 24 | -5.046 | 47.558 | 40.154 | 1.00 | 100.00 |
| ATOM | 181 | NH1 | ARG | A | 24 | -5.263 | 48.853 | 40.383 | 1.00 | 100.00 |
| ATOM | 182 | NH2 | ARG | A | 24 | -6.104 | 46.743 | 40.069 | 1.00 | 100.00 |
| ATOM | 183 | N   | CYS | A | 25 | -1.426 | 50.431 | 45.031 | 1.00 | 39.47  |
| ATOM | 184 | CA  | CYS | A | 25 | -1.849 | 51.420 | 46.022 | 1.00 | 37.37  |
| ATOM | 185 | C   | CYS | A | 25 | -1.146 | 52.736 | 45.798 | 1.00 | 36.83  |
| ATOM | 186 | O   | CYS | A | 25 | -0.142 | 52.824 | 45.066 | 1.00 | 33.74  |
| ATOM | 187 | CB  | CYS | A | 25 | -1.530 | 50.963 | 47.475 | 1.00 | 35.76  |
| ATOM | 188 | SG  | CYS | A | 25 | 0.259  | 50.957 | 47.818 | 1.00 | 38.00  |
| ATOM | 189 | N   | SER | A | 26 | -1.713 | 53.740 | 46.463 | 1.00 | 36.43  |
| ATOM | 190 | CA  | SER | A | 26 | -1.142 | 55.075 | 46.417 | 1.00 | 38.33  |
| ATOM | 191 | C   | SER | A | 26 | -0.971 | 55.634 | 47.816 | 1.00 | 30.93  |
| ATOM | 192 | O   | SER | A | 26 | -1.815 | 55.443 | 48.713 | 1.00 | 29.52  |
| ATOM | 193 | CB  | SER | A | 26 | -1.828 | 56.089 | 45.502 | 1.00 | 49.53  |
| ATOM | 194 | OG  | SER | A | 26 | -0.941 | 57.173 | 45.231 | 1.00 | 58.28  |
| ATOM | 195 | N   | VAL | A | 27 | 0.151  | 56.326 | 47.925 | 1.00 | 30.23  |
| ATOM | 196 | CA  | VAL | A | 27 | 0.555  | 56.974 | 49.156 | 1.00 | 31.98  |
| ATOM | 197 | C   | VAL | A | 27 | 0.120  | 58.438 | 49.259 | 1.00 | 34.81  |
| ATOM | 198 | O   | VAL | A | 27 | 0.708  | 59.320 | 48.614 | 1.00 | 36.20  |
| ATOM | 199 | CB  | VAL | A | 27 | 2.056  | 56.797 | 49.389 | 1.00 | 36.39  |
| ATOM | 200 | CG1 | VAL | A | 27 | 2.402  | 57.292 | 50.802 | 1.00 | 36.16  |
| ATOM | 201 | CG2 | VAL | A | 27 | 2.392  | 55.309 | 49.226 | 1.00 | 34.26  |
| ATOM | 202 | N   | ASP | A | 28 | -0.915 | 58.693 | 50.070 | 1.00 | 32.47  |
| ATOM | 203 | CA  | ASP | A | 28 | -1.391 | 60.061 | 50.283 | 1.00 | 32.12  |
| ATOM | 204 | C   | ASP | A | 28 | -0.872 | 60.655 | 51.590 | 1.00 | 29.94  |
| ATOM | 205 | O   | ASP | A | 28 | -1.385 | 60.375 | 52.668 | 1.00 | 27.16  |
| ATOM | 206 | CB  | ASP | A | 28 | -2.908 | 60.186 | 50.345 | 1.00 | 35.00  |
| ATOM | 207 | CG  | ASP | A | 28 | -3.313 | 61.619 | 50.120 | 1.00 | 53.22  |
| ATOM | 208 | OD1 | ASP | A | 28 | -2.651 | 62.584 | 50.471 | 1.00 | 49.41  |
| ATOM | 209 | OD2 | ASP | A | 28 | -4.427 | 61.711 | 49.443 | 1.00 | 71.15  |
| ATOM | 210 | N   | PHE | A | 29 | 0.151  | 61.476 | 51.445 | 1.00 | 26.90  |
| ATOM | 211 | CA  | PHE | A | 29 | 0.824  | 62.141 | 52.517 | 1.00 | 30.95  |
| ATOM | 212 | C   | PHE | A | 29 | 0.030  | 63.292 | 53.087 | 1.00 | 46.44  |
| ATOM | 213 | O   | PHE | A | 29 | 0.319  | 63.796 | 54.155 | 1.00 | 49.29  |
| ATOM | 214 | CB  | PHE | A | 29 | 2.100  | 62.723 | 51.935 | 1.00 | 35.58  |
| ATOM | 215 | CG  | PHE | A | 29 | 3.276  | 61.805 | 52.080 | 1.00 | 42.10  |
| ATOM | 216 | CD1 | PHE | A | 29 | 3.676  | 61.428 | 53.360 | 1.00 | 46.10  |
| ATOM | 217 | CD2 | PHE | A | 29 | 3.981  | 61.318 | 50.978 | 1.00 | 48.22  |
| ATOM | 218 | CE1 | PHE | A | 29 | 4.765  | 60.586 | 53.561 | 1.00 | 44.91  |



|      |     |     |     |   |    |        |        |        |      |       |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|
| ATOM | 219 | CE2 | PHE | A | 29 | 5.073  | 60.468 | 51.159 | 1.00 | 52.10 |
| ATOM | 220 | CZ  | PHE | A | 29 | 5.465  | 60.115 | 52.451 | 1.00 | 47.34 |
| ATOM | 221 | N   | THR | A | 30 | -0.968 | 63.747 | 52.360 | 1.00 | 48.35 |
| ATOM | 222 | CA  | THR | A | 30 | -1.739 | 64.842 | 52.861 | 1.00 | 45.84 |
| ATOM | 223 | C   | THR | A | 30 | -2.775 | 64.261 | 53.763 | 1.00 | 44.97 |
| ATOM | 224 | O   | THR | A | 30 | -3.096 | 64.772 | 54.823 | 1.00 | 49.48 |
| ATOM | 225 | CB  | THR | A | 30 | -2.404 | 65.608 | 51.725 | 1.00 | 55.54 |
| ATOM | 226 | OG1 | THR | A | 30 | -1.559 | 66.700 | 51.398 | 1.00 | 68.26 |
| ATOM | 227 | CG2 | THR | A | 30 | -3.777 | 66.061 | 52.205 | 1.00 | 46.96 |
| ATOM | 228 | N   | ARG | A | 31 | -3.283 | 63.147 | 53.323 | 1.00 | 32.80 |
| ATOM | 229 | CA  | ARG | A | 31 | -4.268 | 62.480 | 54.132 | 1.00 | 32.20 |
| ATOM | 230 | C   | ARG | A | 31 | -3.634 | 61.456 | 55.067 | 1.00 | 32.13 |
| ATOM | 231 | O   | ARG | A | 31 | -4.409 | 60.864 | 55.817 | 1.00 | 25.23 |
| ATOM | 232 | CB  | ARG | A | 31 | -5.159 | 61.629 | 53.241 | 1.00 | 35.88 |
| ATOM | 233 | CG  | ARG | A | 31 | -6.462 | 62.306 | 52.863 | 1.00 | 66.91 |
| ATOM | 234 | CD  | ARG | A | 31 | -6.539 | 62.672 | 51.392 | 1.00 | 93.56 |
| ATOM | 235 | NE  | ARG | A | 31 | -5.721 | 63.825 | 51.011 | 1.00 | 98.33 |
| ATOM | 236 | CZ  | ARG | A | 31 | -6.218 | 64.857 | 50.328 | 1.00 | 89.65 |
| ATOM | 237 | NH1 | ARG | A | 31 | -7.498 | 64.895 | 49.977 | 1.00 | 51.14 |
| ATOM | 238 | NH2 | ARG | A | 31 | -5.436 | 65.878 | 49.985 | 1.00 | 74.59 |
| ATOM | 239 | N   | ARG | A | 32 | -2.297 | 61.231 | 54.941 | 1.00 | 31.30 |
| ATOM | 240 | CA  | ARG | A | 32 | -1.532 | 60.215 | 55.692 | 1.00 | 32.00 |
| ATOM | 241 | C   | ARG | A | 32 | -2.237 | 58.877 | 55.522 | 1.00 | 35.90 |
| ATOM | 242 | O   | ARG | A | 32 | -2.616 | 58.213 | 56.497 | 1.00 | 26.95 |
| ATOM | 243 | CB  | ARG | A | 32 | -1.207 | 60.481 | 57.169 | 1.00 | 26.70 |
| ATOM | 244 | CG  | ARG | A | 32 | -1.154 | 61.960 | 57.566 | 1.00 | 62.26 |
| ATOM | 245 | CD  | ARG | A | 32 | 0.170  | 62.511 | 58.124 | 1.00 | 84.61 |
| ATOM | 246 | NE  | ARG | A | 32 | 0.480  | 62.134 | 59.510 | 1.00 | 72.60 |
| ATOM | 247 | CZ  | ARG | A | 32 | 1.452  | 62.642 | 60.280 | 1.00 | 62.89 |
| ATOM | 248 | NH1 | ARG | A | 32 | 2.263  | 63.606 | 59.881 | 1.00 | 47.22 |
| ATOM | 249 | NH2 | ARG | A | 32 | 1.636  | 62.159 | 61.505 | 1.00 | 34.21 |
| ATOM | 250 | N   | THR | A | 33 | -2.450 | 58.522 | 54.252 | 1.00 | 32.05 |
| ATOM | 251 | CA  | THR | A | 33 | -3.137 | 57.281 | 53.939 | 1.00 | 31.81 |
| ATOM | 252 | C   | THR | A | 33 | -2.518 | 56.516 | 52.788 | 1.00 | 38.17 |
| ATOM | 253 | O   | THR | A | 33 | -1.863 | 57.045 | 51.884 | 1.00 | 40.95 |
| ATOM | 254 | CB  | THR | A | 33 | -4.604 | 57.441 | 53.507 | 1.00 | 40.71 |
| ATOM | 255 | OG1 | THR | A | 33 | -4.727 | 58.394 | 52.471 | 1.00 | 49.59 |
| ATOM | 256 | CG2 | THR | A | 33 | -5.598 | 57.635 | 54.638 | 1.00 | 36.31 |
| ATOM | 257 | N   | LEU | A | 34 | -2.804 | 55.231 | 52.887 | 1.00 | 36.61 |
| ATOM | 258 | CA  | LEU | A | 34 | -2.446 | 54.238 | 51.916 | 1.00 | 37.65 |
| ATOM | 259 | C   | LEU | A | 34 | -3.787 | 53.723 | 51.432 | 1.00 | 30.48 |
| ATOM | 260 | O   | LEU | A | 34 | -4.667 | 53.249 | 52.175 | 1.00 | 31.53 |
| ATOM | 261 | CB  | LEU | A | 34 | -1.595 | 53.099 | 52.497 | 1.00 | 39.99 |
| ATOM | 262 | CG  | LEU | A | 34 | -0.159 | 53.091 | 52.033 | 1.00 | 44.09 |
| ATOM | 263 | CD1 | LEU | A | 34 | 0.279  | 51.634 | 52.017 | 1.00 | 42.13 |
| ATOM | 264 | CD2 | LEU | A | 34 | -0.102 | 53.656 | 50.627 | 1.00 | 52.70 |
| ATOM | 265 | N   | THR | A | 35 | -3.963 | 53.889 | 50.149 | 1.00 | 29.30 |
| ATOM | 266 | CA  | THR | A | 35 | -5.230 | 53.461 | 49.625 | 1.00 | 34.60 |
| ATOM | 267 | C   | THR | A | 35 | -5.039 | 52.558 | 48.420 | 1.00 | 39.30 |
| ATOM | 268 | O   | THR | A | 35 | -4.116 | 52.754 | 47.594 | 1.00 | 36.72 |
| ATOM | 269 | CB  | THR | A | 35 | -5.983 | 54.705 | 49.146 | 1.00 | 62.16 |
| ATOM | 270 | OG1 | THR | A | 35 | -6.129 | 55.655 | 50.184 | 1.00 | 63.09 |
| ATOM | 271 | CG2 | THR | A | 35 | -7.320 | 54.270 | 48.569 | 1.00 | 67.46 |
| ATOM | 272 | N   | GLY | A | 36 | -5.923 | 51.576 | 48.315 | 1.00 | 33.04 |
| ATOM | 273 | CA  | GLY | A | 36 | -5.736 | 50.731 | 47.162 | 1.00 | 32.58 |
| ATOM | 274 | C   | GLY | A | 36 | -6.472 | 49.414 | 47.226 | 1.00 | 29.34 |
| ATOM | 275 | O   | GLY | A | 36 | -7.502 | 49.276 | 47.901 | 1.00 | 29.27 |
| ATOM | 276 | N   | THR | A | 37 | -5.871 | 48.454 | 46.512 | 1.00 | 29.27 |



|      |     |     |     |   |    |        |        |        |      |       |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|
| ATOM | 277 | CA  | THR | A | 37 | -6.422 | 47.099 | 46.445 | 1.00 | 30.12 |
| ATOM | 278 | C   | THR | A | 37 | -5.399 | 46.039 | 46.733 | 1.00 | 27.15 |
| ATOM | 279 | O   | THR | A | 37 | -4.260 | 46.093 | 46.280 | 1.00 | 29.53 |
| ATOM | 280 | CB  | THR | A | 37 | -6.985 | 46.710 | 45.065 | 1.00 | 29.58 |
| ATOM | 281 | OG1 | THR | A | 37 | -6.019 | 47.050 | 44.078 | 1.00 | 35.41 |
| ATOM | 282 | CG2 | THR | A | 37 | -8.267 | 47.478 | 44.850 | 1.00 | 34.18 |
| ATOM | 283 | N   | ALA | A | 38 | -5.911 | 45.069 | 47.445 | 1.00 | 25.51 |
| ATOM | 284 | CA  | ALA | A | 38 | -5.117 | 43.938 | 47.811 | 1.00 | 28.59 |
| ATOM | 285 | C   | ALA | A | 38 | -5.727 | 42.723 | 47.142 | 1.00 | 28.95 |
| ATOM | 286 | O   | ALA | A | 38 | -6.743 | 42.181 | 47.580 | 1.00 | 29.76 |
| ATOM | 287 | CB  | ALA | A | 38 | -5.053 | 43.783 | 49.332 | 1.00 | 28.09 |
| ATOM | 288 | N   | ALA | A | 39 | -5.087 | 42.281 | 46.069 | 1.00 | 29.16 |
| ATOM | 289 | CA  | ALA | A | 39 | -5.595 | 41.098 | 45.400 | 1.00 | 28.96 |
| ATOM | 290 | C   | ALA | A | 39 | -4.856 | 39.897 | 45.952 | 1.00 | 32.32 |
| ATOM | 291 | O   | ALA | A | 39 | -3.656 | 39.721 | 45.724 | 1.00 | 31.17 |
| ATOM | 292 | CB  | ALA | A | 39 | -5.360 | 41.169 | 43.908 | 1.00 | 28.71 |
| ATOM | 293 | N   | LEU | A | 40 | -5.592 | 39.103 | 46.706 | 1.00 | 29.20 |
| ATOM | 294 | CA  | LEU | A | 40 | -5.003 | 37.945 | 47.317 | 1.00 | 30.98 |
| ATOM | 295 | C   | LEU | A | 40 | -5.327 | 36.648 | 46.592 | 1.00 | 34.18 |
| ATOM | 296 | O   | LEU | A | 40 | -6.498 | 36.316 | 46.393 | 1.00 | 32.36 |
| ATOM | 297 | CB  | LEU | A | 40 | -5.554 | 37.761 | 48.760 | 1.00 | 31.07 |
| ATOM | 298 | CG  | LEU | A | 40 | -5.397 | 38.943 | 49.718 | 1.00 | 31.64 |
| ATOM | 299 | CD1 | LEU | A | 40 | -5.822 | 38.486 | 51.108 | 1.00 | 28.47 |
| ATOM | 300 | CD2 | LEU | A | 40 | -3.944 | 39.386 | 49.725 | 1.00 | 21.87 |
| ATOM | 301 | N   | THR | A | 41 | -4.311 | 35.861 | 46.263 | 1.00 | 30.21 |
| ATOM | 302 | CA  | THR | A | 41 | -4.632 | 34.568 | 45.683 | 1.00 | 30.42 |
| ATOM | 303 | C   | THR | A | 41 | -4.602 | 33.586 | 46.837 | 1.00 | 35.30 |
| ATOM | 304 | O   | THR | A | 41 | -3.571 | 33.422 | 47.482 | 1.00 | 34.05 |
| ATOM | 305 | CB  | THR | A | 41 | -3.679 | 34.105 | 44.584 | 1.00 | 42.24 |
| ATOM | 306 | OG1 | THR | A | 41 | -3.701 | 35.078 | 43.562 | 1.00 | 39.08 |
| ATOM | 307 | CG2 | THR | A | 41 | -4.097 | 32.709 | 44.090 | 1.00 | 29.36 |
| ATOM | 308 | N   | VAL | A | 42 | -5.752 | 32.982 | 47.091 | 1.00 | 30.50 |
| ATOM | 309 | CA  | VAL | A | 42 | -5.944 | 32.058 | 48.180 | 1.00 | 30.58 |
| ATOM | 310 | C   | VAL | A | 42 | -6.186 | 30.625 | 47.728 | 1.00 | 38.17 |
| ATOM | 311 | O   | VAL | A | 42 | -6.913 | 30.370 | 46.764 | 1.00 | 37.98 |
| ATOM | 312 | CB  | VAL | A | 42 | -7.074 | 32.551 | 49.091 | 1.00 | 31.60 |
| ATOM | 313 | CG1 | VAL | A | 42 | -7.339 | 31.536 | 50.190 | 1.00 | 30.16 |
| ATOM | 314 | CG2 | VAL | A | 42 | -6.681 | 33.877 | 49.750 | 1.00 | 31.76 |
| ATOM | 315 | N   | GLN | A | 43 | -5.570 | 29.690 | 48.453 | 1.00 | 30.27 |
| ATOM | 316 | CA  | GLN | A | 43 | -5.721 | 28.291 | 48.163 | 1.00 | 28.24 |
| ATOM | 317 | C   | GLN | A | 43 | -6.374 | 27.521 | 49.293 | 1.00 | 30.98 |
| ATOM | 318 | O   | GLN | A | 43 | -5.906 | 27.495 | 50.437 | 1.00 | 30.47 |
| ATOM | 319 | CB  | GLN | A | 43 | -4.376 | 27.685 | 47.751 | 1.00 | 30.68 |
| ATOM | 320 | CG  | GLN | A | 43 | -4.447 | 26.152 | 47.645 | 1.00 | 44.61 |



|      |     |     |     |   |    |         |        |        |      |        |
|------|-----|-----|-----|---|----|---------|--------|--------|------|--------|
| ATOM | 335 | CG  | GLN | A | 45 | -5.209  | 24.589 | 53.105 | 1.00 | 19.22  |
| ATOM | 336 | CD  | GLN | A | 45 | -4.264  | 24.414 | 51.939 | 1.00 | 44.80  |
| ATOM | 337 | OE1 | GLN | A | 45 | -4.199  | 25.228 | 50.995 | 1.00 | 46.26  |
| ATOM | 338 | NE2 | GLN | A | 45 | -3.520  | 23.319 | 52.002 | 1.00 | 28.67  |
| ATOM | 339 | N   | GLU | A | 46 | -9.295  | 22.622 | 52.280 | 1.00 | 38.36  |
| ATOM | 340 | CA  | GLU | A | 46 | -10.494 | 21.931 | 52.674 | 1.00 | 41.96  |
| ATOM | 341 | C   | GLU | A | 46 | -11.465 | 21.892 | 51.512 | 1.00 | 44.78  |
| ATOM | 342 | O   | GLU | A | 46 | -11.482 | 22.772 | 50.648 | 1.00 | 38.52  |
| ATOM | 343 | CB  | GLU | A | 46 | -11.225 | 22.681 | 53.828 | 1.00 | 44.36  |
| ATOM | 344 | CG  | GLU | A | 46 | -10.440 | 22.959 | 55.132 | 1.00 | 56.09  |
| ATOM | 345 | CD  | GLU | A | 46 | -11.309 | 23.520 | 56.226 | 1.00 | 70.52  |
| ATOM | 346 | OE1 | GLU | A | 46 | -12.359 | 24.099 | 55.997 | 1.00 | 65.91  |
| ATOM | 347 | OE2 | GLU | A | 46 | -10.822 | 23.315 | 57.432 | 1.00 | 89.95  |
| ATOM | 348 | N   | ASP | A | 47 | -12.301 | 20.871 | 51.516 | 1.00 | 45.87  |
| ATOM | 349 | CA  | ASP | A | 47 | -13.287 | 20.831 | 50.474 | 1.00 | 49.24  |
| ATOM | 350 | C   | ASP | A | 47 | -14.443 | 21.658 | 50.966 | 1.00 | 50.94  |
| ATOM | 351 | O   | ASP | A | 47 | -14.693 | 21.733 | 52.167 | 1.00 | 50.75  |
| ATOM | 352 | CB  | ASP | A | 47 | -13.770 | 19.400 | 50.251 | 1.00 | 53.61  |
| ATOM | 353 | CG  | ASP | A | 47 | -12.685 | 18.588 | 49.621 | 1.00 | 74.24  |
| ATOM | 354 | OD1 | ASP | A | 47 | -12.004 | 19.005 | 48.689 | 1.00 | 70.46  |
| ATOM | 355 | OD2 | ASP | A | 47 | -12.545 | 17.420 | 50.206 | 1.00 | 90.87  |
| ATOM | 356 | N   | ASN | A | 48 | -15.152 | 22.285 | 50.059 | 1.00 | 48.17  |
| ATOM | 357 | CA  | ASN | A | 48 | -16.290 | 23.066 | 50.491 | 1.00 | 48.03  |
| ATOM | 358 | C   | ASN | A | 48 | -15.954 | 24.303 | 51.298 | 1.00 | 44.92  |
| ATOM | 359 | O   | ASN | A | 48 | -16.641 | 24.644 | 52.272 | 1.00 | 40.67  |
| ATOM | 360 | CB  | ASN | A | 48 | -17.289 | 22.225 | 51.310 | 1.00 | 44.29  |
| ATOM | 361 | CG  | ASN | A | 48 | -18.688 | 22.771 | 51.105 | 1.00 | 86.53  |
| ATOM | 362 | OD1 | ASN | A | 48 | -19.012 | 23.236 | 49.996 | 1.00 | 80.31  |
| ATOM | 363 | ND2 | ASN | A | 48 | -19.495 | 22.754 | 52.167 | 1.00 | 79.87  |
| ATOM | 364 | N   | LEU | A | 49 | -14.902 | 24.975 | 50.899 | 1.00 | 37.27  |
| ATOM | 365 | CA  | LEU | A | 49 | -14.575 | 26.165 | 51.639 | 1.00 | 35.59  |
| ATOM | 366 | C   | LEU | A | 49 | -15.499 | 27.253 | 51.115 | 1.00 | 40.36  |
| ATOM | 367 | O   | LEU | A | 49 | -15.408 | 27.618 | 49.944 | 1.00 | 41.04  |
| ATOM | 368 | CB  | LEU | A | 49 | -13.075 | 26.504 | 51.519 | 1.00 | 33.17  |
| ATOM | 369 | CG  | LEU | A | 49 | -12.645 | 27.780 | 52.244 | 1.00 | 36.35  |
| ATOM | 370 | CD1 | LEU | A | 49 | -12.842 | 27.583 | 53.737 | 1.00 | 34.98  |
| ATOM | 371 | CD2 | LEU | A | 49 | -11.169 | 28.024 | 51.977 | 1.00 | 32.02  |
| ATOM | 372 | N   | ARG | A | 50 | -16.402 | 27.745 | 51.966 | 1.00 | 38.16  |
| ATOM | 373 | CA  | ARG | A | 50 | -17.343 | 28.785 | 51.541 | 1.00 | 40.98  |
| ATOM | 374 | C   | ARG | A | 50 | -17.066 | 30.228 | 51.997 | 1.00 | 46.66  |
| ATOM | 375 | O   | ARG | A | 50 | -17.541 | 31.214 | 51.410 | 1.00 | 38.00  |
| ATOM | 376 | CB  | ARG | A | 50 | -18.744 | 28.339 | 51.902 | 1.00 | 46.12  |
| ATOM | 377 | CG  | ARG | A | 50 | -19.238 | 27.266 | 50.932 | 1.00 | 61.10  |
| ATOM | 378 | CD  | ARG | A | 50 | -20.306 | 26.345 | 51.511 | 1.00 | 75.76  |
| ATOM | 379 | NE  | ARG | A | 50 | -20.745 | 25.322 | 50.554 | 1.00 | 100.00 |
| ATOM | 380 | CZ  | ARG | A | 50 | -21.979 | 24.809 | 50.451 | 1.00 | 100.00 |
| ATOM | 381 | NH1 | ARG | A | 50 | -22.981 | 25.195 | 51.240 | 1.00 | 100.00 |
| ATOM | 382 | NH2 | ARG | A | 50 | -22.220 | 23.875 | 49.527 | 1.00 | 84.13  |
| ATOM | 383 | N   | SER | A | 51 | -16.271 | 30.339 | 53.066 | 1.00 | 50.16  |
| ATOM | 384 | CA  | SER | A | 51 | -15.885 | 31.610 | 53.671 | 1.00 | 49.64  |
| ATOM | 385 | C   | SER | A | 51 | -14.550 | 31.540 | 54.403 | 1.00 | 47.77  |
| ATOM | 386 | O   | SER | A | 51 | -14.207 | 30.522 | 55.029 | 1.00 | 42.04  |
| ATOM | 387 | CB  | SER | A | 51 | -16.925 | 32.073 | 54.697 | 1.00 | 53.65  |
| ATOM | 388 | OG  | SER | A | 51 | -17.107 | 31.125 | 55.755 | 1.00 | 51.47  |
| ATOM | 389 | N   | LEU | A | 52 | -13.829 | 32.663 | 54.351 | 1.00 | 41.55  |
| ATOM | 390 | CA  | LEU | A | 52 | -12.575 | 32.757 | 55.087 | 1.00 | 40.56  |
| ATOM | 391 | C   | LEU | A | 52 | -12.474 | 33.996 | 55.991 | 1.00 | 43.53  |
| ATOM | 392 | O   | LEU | A | 52 | -13.288 | 34.921 | 55.895 | 1.00 | 39.84  |



|      |     |     |     |   |    |         |        |        |      |       |
|------|-----|-----|-----|---|----|---------|--------|--------|------|-------|
| ATOM | 393 | CB  | LEU | A | 52 | -11.291 | 32.385 | 54.325 | 1.00 | 39.23 |
| ATOM | 394 | CG  | LEU | A | 52 | -10.884 | 33.281 | 53.164 | 1.00 | 45.23 |
| ATOM | 395 | CD1 | LEU | A | 52 | -11.692 | 32.934 | 51.927 | 1.00 | 47.83 |
| ATOM | 396 | CD2 | LEU | A | 52 | -10.973 | 34.762 | 53.516 | 1.00 | 44.42 |
| ATOM | 397 | N   | VAL | A | 53 | -11.489 | 34.013 | 56.899 | 1.00 | 37.60 |
| ATOM | 398 | CA  | VAL | A | 53 | -11.289 | 35.157 | 57.773 | 1.00 | 32.60 |
| ATOM | 399 | C   | VAL | A | 53 | -9.902  | 35.696 | 57.554 | 1.00 | 31.28 |
| ATOM | 400 | O   | VAL | A | 53 | -8.942  | 34.925 | 57.414 | 1.00 | 26.57 |
| ATOM | 401 | CB  | VAL | A | 53 | -11.527 | 34.916 | 59.258 | 1.00 | 34.90 |
| ATOM | 402 | CG1 | VAL | A | 53 | -11.411 | 36.227 | 60.052 | 1.00 | 32.09 |
| ATOM | 403 | CG2 | VAL | A | 53 | -12.904 | 34.310 | 59.444 | 1.00 | 34.64 |
| ATOM | 404 | N   | LEU | A | 54 | -9.857  | 37.020 | 57.478 | 1.00 | 22.73 |
| ATOM | 405 | CA  | LEU | A | 54 | -8.634  | 37.730 | 57.325 | 1.00 | 21.84 |
| ATOM | 406 | C   | LEU | A | 54 | -8.434  | 38.607 | 58.562 | 1.00 | 30.12 |
| ATOM | 407 | O   | LEU | A | 54 | -9.386  | 38.932 | 59.275 | 1.00 | 27.27 |
| ATOM | 408 | CB  | LEU | A | 54 | -8.642  | 38.619 | 56.097 | 1.00 | 23.04 |
| ATOM | 409 | CG  | LEU | A | 54 | -8.545  | 37.839 | 54.796 | 1.00 | 29.10 |
| ATOM | 410 | CD1 | LEU | A | 54 | -8.495  | 38.869 | 53.678 | 1.00 | 26.16 |
| ATOM | 411 | CD2 | LEU | A | 54 | -7.251  | 37.027 | 54.743 | 1.00 | 24.36 |
| ATOM | 412 | N   | ASP | A | 55 | -7.175  | 38.970 | 58.810 | 1.00 | 27.32 |
| ATOM | 413 | CA  | ASP | A | 55 | -6.807  | 39.843 | 59.910 | 1.00 | 24.82 |
| ATOM | 414 | C   | ASP | A | 55 | -6.785  | 41.269 | 59.354 | 1.00 | 24.10 |
| ATOM | 415 | O   | ASP | A | 55 | -6.404  | 41.485 | 58.196 | 1.00 | 20.86 |
| ATOM | 416 | CB  | ASP | A | 55 | -5.390  | 39.545 | 60.475 | 1.00 | 23.73 |
| ATOM | 417 | CG  | ASP | A | 55 | -5.197  | 38.294 | 61.291 | 1.00 | 16.69 |
| ATOM | 418 | OD1 | ASP | A | 55 | -5.748  | 38.060 | 62.371 | 1.00 | 23.25 |
| ATOM | 419 | OD2 | ASP | A | 55 | -4.279  | 37.499 | 60.737 | 1.00 | 20.96 |
| ATOM | 420 | N   | THR | A | 56 | -7.203  | 42.241 | 60.199 | 1.00 | 24.09 |
| ATOM | 421 | CA  | THR | A | 56 | -7.176  | 43.675 | 59.882 | 1.00 | 21.61 |
| ATOM | 422 | C   | THR | A | 56 | -6.990  | 44.475 | 61.175 | 1.00 | 20.13 |
| ATOM | 423 | O   | THR | A | 56 | -7.355  | 44.035 | 62.254 | 1.00 | 18.34 |
| ATOM | 424 | CB  | THR | A | 56 | -8.477  | 44.244 | 59.263 | 1.00 | 21.22 |
| ATOM | 425 | OG1 | THR | A | 56 | -9.507  | 44.197 | 60.246 | 1.00 | 22.90 |
| ATOM | 426 | CG2 | THR | A | 56 | -8.831  | 43.494 | 57.987 | 1.00 | 21.74 |
| ATOM | 427 | N   | LYS | A | 57 | -6.498  | 45.695 | 61.046 | 1.00 | 20.23 |
| ATOM | 428 | CA  | LYS | A | 57 | -6.428  | 46.501 | 62.242 | 1.00 | 19.81 |
| ATOM | 429 | C   | LYS | A | 57 | -6.591  | 47.937 | 61.799 | 1.00 | 21.15 |
| ATOM | 430 | O   | LYS | A | 57 | -5.807  | 48.429 | 61.010 | 1.00 | 19.90 |
| ATOM | 431 | CB  | LYS | A | 57 | -5.124  | 46.230 | 62.926 | 1.00 | 24.68 |
| ATOM | 432 | CG  | LYS | A | 57 | -4.922  | 46.928 | 64.262 | 1.00 | 40.66 |
| ATOM | 433 | CD  | LYS | A | 57 | -3.439  | 47.032 | 64.609 | 1.00 | 42.93 |
| ATOM | 434 | CE  | LYS | A | 57 | -3.141  | 46.702 | 66.060 | 1.00 | 75.78 |
| ATOM | 435 | NZ  | LYS | A | 57 | -1.894  | 47.316 | 66.567 | 1.00 | 94.53 |
| ATOM | 436 | N   | ASP | A | 58 | -7.639  | 48.622 | 62.241 | 1.00 | 20.19 |
| ATOM | 437 | CA  | ASP | A | 58 | -7.788  | 49.989 | 61.784 | 1.00 | 17.85 |
| ATOM | 438 | C   | ASP | A | 58 | -7.836  | 50.124 | 60.283 | 1.00 | 24.95 |
| ATOM | 439 | O   | ASP | A | 58 | -7.335  | 51.088 | 59.678 | 1.00 | 23.25 |
| ATOM | 440 | CB  | ASP | A | 58 | -6.780  | 50.959 | 62.402 | 1.00 | 21.68 |
| ATOM | 441 | CG  | ASP | A | 58 | -7.118  | 50.982 | 63.856 | 1.00 | 36.83 |
| ATOM | 442 | OD1 | ASP | A | 58 | -8.253  | 51.136 | 64.263 | 1.00 | 40.21 |
| ATOM | 443 | OD2 | ASP | A | 58 | -6.100  | 50.683 | 64.618 | 1.00 | 37.52 |
| ATOM | 444 | N   | LEU | A | 59 | -8.466  | 49.121 | 59.698 | 1.00 | 26.52 |
| ATOM | 445 | CA  | LEU | A | 59 | -8.615  | 49.130 | 58.259 | 1.00 | 29.86 |
| ATOM | 446 | C   | LEU | A | 59 | -10.025 | 49.586 | 57.847 | 1.00 | 33.01 |
| ATOM | 447 | O   | LEU | A | 59 | -11.070 | 49.255 | 58.424 | 1.00 | 29.32 |
| ATOM | 448 | CB  | LEU | A | 59 | -8.196  | 47.789 | 57.588 | 1.00 | 29.02 |
| ATOM | 449 | CG  | LEU | A | 59 | -6.682  | 47.520 | 57.589 | 1.00 | 29.22 |
| ATOM | 450 | CD1 | LEU | A | 59 | -6.377  | 46.244 | 56.795 | 1.00 | 29.68 |



|      |     |     |     |   |      |         |        |        |      |        |
|------|-----|-----|-----|---|------|---------|--------|--------|------|--------|
| ATOM | 451 | CD2 | LEU | A | 59   | -5.923  | 48.703 | 56.978 | 1.00 | 22.97  |
| ATOM | 452 | N   | THR | A | 60   | -10.029 | 50.399 | 56.819 | 1.00 | 36.77  |
| ATOM | 453 | CA  | THR | A | 60   | -11.279 | 50.877 | 56.254 | 1.00 | 42.01  |
| ATOM | 454 | C   | THR | A | 60   | -11.494 | 50.092 | 54.940 | 1.00 | 36.44  |
| ATOM | 455 | O   | THR | A | 60   | -10.694 | 50.247 | 53.992 | 1.00 | 33.67  |
| ATOM | 456 | CB  | THR | A | 60   | -11.220 | 52.424 | 56.080 | 1.00 | 56.43  |
| ATOM | 457 | OG1 | THR | A | 60   | -11.614 | 53.107 | 57.261 | 1.00 | 52.66  |
| ATOM | 458 | CG2 | THR | A | 60   | -12.034 | 52.910 | 54.893 | 1.00 | 60.41  |
| ATOM | 459 | N   | ILE | A | 61   | -12.515 | 49.227 | 54.909 | 1.00 | 29.81  |
| ATOM | 460 | CA  | ILE | A | 61   | -12.779 | 48.432 | 53.711 | 1.00 | 32.79  |
| ATOM | 461 | C   | ILE | A | 61   | -13.799 | 49.068 | 52.780 | 1.00 | 35.88  |
| ATOM | 462 | O   | ILE | A | 61   | -14.939 | 49.202 | 53.176 | 1.00 | 30.98  |
| ATOM | 463 | CB  | ILE | A | 61   | -13.337 | 47.038 | 53.972 | 1.00 | 37.74  |
| ATOM | 464 | CG1 | ILE | A | 61   | -12.616 | 46.331 | 55.118 | 1.00 | 40.37  |
| ATOM | 465 | CG2 | ILE | A | 61   | -13.264 | 46.240 | 52.661 | 1.00 | 36.33  |
| ATOM | 466 | CD1 | ILE | A | 61   | -11.098 | 46.353 | 54.952 | 1.00 | 49.83  |
| ATOM | 467 | N   | GLU | A | 62   | -13.396 | 49.409 | 51.562 | 1.00 | 40.08  |
| ATOM | 468 | CA  | GLU | A | 62   | -14.276 | 49.995 | 50.553 | 1.00 | 43.04  |
| ATOM | 469 | C   | GLU | A | 62   | -15.199 | 48.885 | 50.016 | 1.00 | 45.27  |
| ATOM | 470 | O   | GLU | A | 62   | -16.415 | 48.853 | 50.243 | 1.00 | 45.18  |
| ATOM | 471 | CB  | GLU | A | 62   | -13.392 | 50.640 | 49.457 | 1.00 | 45.63  |
| ATOM | 472 | CG  | GLU | A | 62   | -14.131 | 51.580 | 48.471 | 1.00 | 73.11  |
| ATOM | 473 | CD  | GLU | A | 62   | -14.846 | 50.895 | 47.320 | 1.00 | 100.00 |
| ATOM | 474 | OE1 | GLU | A | 62   | -15.037 | 49.689 | 47.286 | 1.00 | 100.00 |
| ATOM | 475 | OE2 | GLU | A | 62   | -15.254 | 51.717 | 46.368 | 1.00 | 100.00 |
| ATOM | 476 | N   | LYS | A | 63   | -14.588 | 47.918 | 49.336 | 1.00 | 38.38  |
| ATOM | 477 | CA  | LYS | A | 63   | -15.311 | 46.761 | 48.838 | 1.00 | 37.37  |
| ATOM | 478 | C   | LYS | A | 63   | -14.396 | 45.541 | 48.702 | 1.00 | 38.22  |
| ATOM | 479 | O   | LYS | A | 63   | -13.167 | 45.646 | 48.717 | 1.00 | 32.45  |
| ATOM | 480 | CB  | LYS | A | 63   | -16.022 | 47.038 | 47.530 | 1.00 | 33.09  |
| ATOM | 481 | CG  | LYS | A | 63   | -15.051 | 47.059 | 46.366 | 1.00 | 27.59  |
| ATOM | 482 | CD  | LYS | A | 63   | -15.548 | 47.905 | 45.207 | 1.00 | 37.24  |
| ATOM | 483 | CE  | LYS | A | 63   | -14.443 | 48.583 | 44.423 | 1.00 | 43.28  |
| ATOM | 484 | NZ  | LYS | A | 63   | -14.395 | 48.151 | 43.015 | 1.00 | 76.13  |
| ATOM | 485 | N   | VAL | A | 64   | -15.049 | 44.395 | 48.574 | 1.00 | 43.49  |
| ATOM | 486 | CA  | VAL | A | 64   | -14.436 | 43.081 | 48.377 | 1.00 | 45.64  |
| ATOM | 487 | C   | VAL | A | 64   | -14.934 | 42.410 | 47.087 | 1.00 | 45.26  |
| ATOM | 488 | O   | VAL | A | 64   | -16.058 | 41.916 | 46.997 | 1.00 | 39.88  |
| ATOM | 489 | CB  | VAL | A | 64   | -14.689 | 42.140 | 49.543 | 1.00 | 48.77  |
| ATOM | 490 | CG1 | VAL | A | 64   | -14.270 | 40.746 | 49.101 | 1.00 | 48.87  |
| ATOM | 491 | CG2 | VAL | A | 64   | -13.861 | 42.572 | 50.742 | 1.00 | 47.38  |
| ATOM | 492 | N   | VAL | A | 65   | -14.096 | 42.380 | 46.077 | 1.00 | 39.08  |
| ATOM | 493 | CA  | VAL | A | 65   | -14.534 | 41.789 | 44.840 | 1.00 | 40.48  |
| ATOM | 494 | C   | VAL | A | 65</ |         |        |        |      |        |



|      |     |     |     |   |    |         |        |        |      |        |
|------|-----|-----|-----|---|----|---------|--------|--------|------|--------|
| ATOM | 509 | C   | ASN | A | 67 | -15.601 | 38.568 | 39.297 | 1.00 | 51.70  |
| ATOM | 510 | O   | ASN | A | 67 | -16.753 | 38.371 | 38.923 | 1.00 | 51.19  |
| ATOM | 511 | CB  | ASN | A | 67 | -15.580 | 36.098 | 39.695 | 1.00 | 32.37  |
| ATOM | 512 | CG  | ASN | A | 67 | -14.756 | 34.862 | 40.037 | 1.00 | 57.02  |
| ATOM | 513 | OD1 | ASN | A | 67 | -13.549 | 34.796 | 39.721 | 1.00 | 42.45  |
| ATOM | 514 | ND2 | ASN | A | 67 | -15.389 | 33.889 | 40.714 | 1.00 | 45.38  |
| ATOM | 515 | N   | GLY | A | 68 | -15.000 | 39.757 | 39.327 | 1.00 | 45.47  |
| ATOM | 516 | CA  | GLY | A | 68 | -15.638 | 40.982 | 38.876 | 1.00 | 44.33  |
| ATOM | 517 | C   | GLY | A | 68 | -16.870 | 41.394 | 39.669 | 1.00 | 52.05  |
| ATOM | 518 | O   | GLY | A | 68 | -17.456 | 42.442 | 39.422 | 1.00 | 60.14  |
| ATOM | 519 | N   | GLN | A | 69 | -17.280 | 40.591 | 40.630 | 1.00 | 45.36  |
| ATOM | 520 | CA  | GLN | A | 69 | -18.458 | 40.930 | 41.403 | 1.00 | 46.40  |
| ATOM | 521 | C   | GLN | A | 69 | -18.156 | 41.109 | 42.894 | 1.00 | 57.29  |
| ATOM | 522 | O   | GLN | A | 69 | -17.404 | 40.355 | 43.525 | 1.00 | 55.55  |
| ATOM | 523 | CB  | GLN | A | 69 | -19.575 | 39.858 | 41.258 | 1.00 | 48.27  |
| ATOM | 524 | CG  | GLN | A | 69 | -20.184 | 39.636 | 39.841 | 1.00 | 33.05  |
| ATOM | 525 | CD  | GLN | A | 69 | -20.435 | 40.926 | 39.098 | 1.00 | 73.86  |
| ATOM | 526 | OE1 | GLN | A | 69 | -19.771 | 41.195 | 38.074 | 1.00 | 70.10  |
| ATOM | 527 | NE2 | GLN | A | 69 | -21.364 | 41.729 | 39.634 | 1.00 | 75.78  |
| ATOM | 528 | N   | GLU | A | 70 | -18.800 | 42.114 | 43.469 | 1.00 | 54.73  |
| ATOM | 529 | CA  | GLU | A | 70 | -18.661 | 42.408 | 44.879 | 1.00 | 53.61  |
| ATOM | 530 | C   | GLU | A | 70 | -19.274 | 41.297 | 45.728 | 1.00 | 54.45  |
| ATOM | 531 | O   | GLU | A | 70 | -20.285 | 40.708 | 45.342 | 1.00 | 56.71  |
| ATOM | 532 | CB  | GLU | A | 70 | -19.244 | 43.794 | 45.191 | 1.00 | 54.16  |
| ATOM | 533 | CG  | GLU | A | 70 | -18.670 | 44.845 | 44.223 | 1.00 | 66.60  |
| ATOM | 534 | CD  | GLU | A | 70 | -19.042 | 46.248 | 44.614 | 1.00 | 99.90  |
| ATOM | 535 | OE1 | GLU | A | 70 | -19.763 | 46.518 | 45.567 | 1.00 | 55.96  |
| ATOM | 536 | OE2 | GLU | A | 70 | -18.515 | 47.139 | 43.807 | 1.00 | 100.00 |
| ATOM | 537 | N   | VAL | A | 71 | -18.652 | 40.992 | 46.875 | 1.00 | 41.84  |
| ATOM | 538 | CA  | VAL | A | 71 | -19.146 | 39.929 | 47.731 | 1.00 | 37.89  |
| ATOM | 539 | C   | VAL | A | 71 | -19.472 | 40.373 | 49.160 | 1.00 | 37.87  |
| ATOM | 540 | O   | VAL | A | 71 | -19.112 | 41.469 | 49.586 | 1.00 | 34.22  |
| ATOM | 541 | CB  | VAL | A | 71 | -18.254 | 38.677 | 47.618 | 1.00 | 41.06  |
| ATOM | 542 | CG1 | VAL | A | 71 | -17.823 | 38.468 | 46.158 | 1.00 | 38.37  |
| ATOM | 543 | CG2 | VAL | A | 71 | -17.012 | 38.800 | 48.500 | 1.00 | 39.32  |
| ATOM | 544 | N   | LYS | A | 72 | -20.182 | 39.513 | 49.897 | 1.00 | 35.47  |
| ATOM | 545 | CA  | LYS | A | 72 | -20.559 | 39.775 | 51.274 | 1.00 | 36.55  |
| ATOM | 546 | C   | LYS | A | 72 | -19.325 | 39.664 | 52.171 | 1.00 | 48.55  |
| ATOM | 547 | O   | LYS | A | 72 | -18.411 | 38.849 | 51.947 | 1.00 | 44.75  |
| ATOM | 548 | CB  | LYS | A | 72 | -21.607 | 38.799 | 51.783 | 1.00 | 36.22  |
| ATOM | 549 | CG  | LYS | A | 72 | -22.618 | 39.411 | 52.729 | 1.00 | 71.24  |
| ATOM | 550 | CD  | LYS | A | 72 | -23.875 | 39.881 | 52.015 | 1.00 | 91.55  |
| ATOM | 551 | CE  | LYS | A | 72 | -25.018 | 40.175 | 52.979 | 1.00 | 100.00 |
| ATOM | 552 | NZ  | LYS | A | 72 | -25.393 | 39.021 | 53.821 | 1.00 | 100.00 |
| ATOM | 553 | N   | TYR | A | 73 | -19.327 | 40.506 | 53.199 | 1.00 | 46.72  |
| ATOM | 554 | CA  | TYR | A | 73 | -18.263 | 40.517 | 54.177 | 1.00 | 46.48  |
| ATOM | 555 | C   | TYR | A | 73 | -18.637 | 41.190 | 55.466 | 1.00 | 47.06  |
| ATOM | 556 | O   | TYR | A | 73 | -19.583 | 41.962 | 55.569 | 1.00 | 46.31  |
| ATOM | 557 | CB  | TYR | A | 73 | -16.956 | 41.091 | 53.662 | 1.00 | 43.25  |
| ATOM | 558 | CG  | TYR | A | 73 | -16.940 | 42.580 | 53.611 | 1.00 | 47.55  |
| ATOM | 559 | CD1 | TYR | A | 73 | -16.675 | 43.327 | 54.752 | 1.00 | 49.47  |
| ATOM | 560 | CD2 | TYR | A | 73 | -17.111 | 43.242 | 52.396 | 1.00 | 49.40  |
| ATOM | 561 | CE1 | TYR | A | 73 | -16.632 | 44.722 | 54.702 | 1.00 | 45.81  |
| ATOM | 562 | CE2 | TYR | A | 73 | -17.031 | 44.632 | 52.315 | 1.00 | 50.44  |
| ATOM | 563 | CZ  | TYR | A | 73 | -16.821 | 45.357 | 53.475 | 1.00 | 55.67  |
| ATOM | 564 | OH  | TYR | A | 73 | -16.761 | 46.722 | 53.409 | 1.00 | 61.06  |
| ATOM | 565 | N   | ALA | A | 74 | -17.852 | 40.860 | 56.462 | 1.00 | 41.61  |
| ATOM | 566 | CA  | ALA | A | 74 | -18.079 | 41.415 | 57.772 | 1.00 | 41.55  |



|      |     |     |     |   |    |         |        |        |      |        |
|------|-----|-----|-----|---|----|---------|--------|--------|------|--------|
| ATOM | 567 | C   | ALA | A | 74 | -16.763 | 41.674 | 58.524 | 1.00 | 45.67  |
| ATOM | 568 | O   | ALA | A | 74 | -15.710 | 41.092 | 58.249 | 1.00 | 38.74  |
| ATOM | 569 | CB  | ALA | A | 74 | -19.074 | 40.572 | 58.563 | 1.00 | 39.69  |
| ATOM | 570 | N   | LEU | A | 75 | -16.861 | 42.609 | 59.464 | 1.00 | 43.41  |
| ATOM | 571 | CA  | LEU | A | 75 | -15.798 | 43.026 | 60.355 | 1.00 | 38.66  |
| ATOM | 572 | C   | LEU | A | 75 | -16.241 | 42.750 | 61.778 | 1.00 | 34.64  |
| ATOM | 573 | O   | LEU | A | 75 | -17.202 | 43.316 | 62.260 | 1.00 | 39.67  |
| ATOM | 574 | CB  | LEU | A | 75 | -15.432 | 44.499 | 60.117 | 1.00 | 38.89  |
| ATOM | 575 | CG  | LEU | A | 75 | -14.504 | 44.657 | 58.913 | 1.00 | 47.18  |
| ATOM | 576 | CD1 | LEU | A | 75 | -14.025 | 46.099 | 58.824 | 1.00 | 51.19  |
| ATOM | 577 | CD2 | LEU | A | 75 | -13.278 | 43.760 | 59.032 | 1.00 | 48.20  |
| ATOM | 578 | N   | GLY | A | 76 | -15.616 | 41.817 | 62.458 | 1.00 | 33.98  |
| ATOM | 579 | CA  | GLY | A | 76 | -16.005 | 41.518 | 63.823 | 1.00 | 34.06  |
| ATOM | 580 | C   | GLY | A | 76 | -15.526 | 42.623 | 64.766 | 1.00 | 38.57  |
| ATOM | 581 | O   | GLY | A | 76 | -14.887 | 43.617 | 64.372 | 1.00 | 36.37  |
| ATOM | 582 | N   | GLU | A | 77 | -15.857 | 42.491 | 66.037 | 1.00 | 38.70  |
| ATOM | 583 | CA  | GLU | A | 77 | -15.395 | 43.560 | 66.900 | 1.00 | 41.69  |
| ATOM | 584 | C   | GLU | A | 77 | -13.907 | 43.415 | 67.146 | 1.00 | 41.16  |
| ATOM | 585 | O   | GLU | A | 77 | -13.371 | 42.308 | 67.121 | 1.00 | 33.89  |
| ATOM | 586 | CB  | GLU | A | 77 | -16.152 | 43.651 | 68.238 | 1.00 | 44.95  |
| ATOM | 587 | CG  | GLU | A | 77 | -16.634 | 42.290 | 68.792 | 1.00 | 66.34  |
| ATOM | 588 | CD  | GLU | A | 77 | -16.713 | 42.271 | 70.307 | 1.00 | 100.00 |
| ATOM | 589 | OE1 | GLU | A | 77 | -16.003 | 41.551 | 71.002 | 1.00 | 100.00 |
| ATOM | 590 | OE2 | GLU | A | 77 | -17.607 | 43.109 | 70.802 | 1.00 | 100.00 |
| ATOM | 591 | N   | ARG | A | 78 | -13.266 | 44.551 | 67.393 | 1.00 | 42.48  |
| ATOM | 592 | CA  | ARG | A | 78 | -11.843 | 44.608 | 67.681 | 1.00 | 40.23  |
| ATOM | 593 | C   | ARG | A | 78 | -11.440 | 43.802 | 68.895 | 1.00 | 38.54  |
| ATOM | 594 | O   | ARG | A | 78 | -12.137 | 43.783 | 69.908 | 1.00 | 33.87  |
| ATOM | 595 | CB  | ARG | A | 78 | -11.360 | 46.010 | 67.939 | 1.00 | 39.17  |
| ATOM | 596 | CG  | ARG | A | 78 | -9.927  | 46.212 | 67.462 | 1.00 | 46.74  |
| ATOM | 597 | CD  | ARG | A | 78 | -9.391  | 47.489 | 68.064 | 1.00 | 34.80  |
| ATOM | 598 | NE  | ARG | A | 78 | -7.960  | 47.579 | 68.004 | 1.00 | 30.05  |
| ATOM | 599 | CZ  | ARG | A | 78 | -7.466  | 48.544 | 67.282 | 1.00 | 56.07  |
| ATOM | 600 | NH1 | ARG | A | 78 | -8.293  | 49.370 | 66.631 | 1.00 | 53.51  |
| ATOM | 601 | NH2 | ARG | A | 78 | -6.144  | 48.657 | 67.205 | 1.00 | 33.42  |
| ATOM | 602 | N   | GLN | A | 79 | -10.293 | 43.133 | 68.761 | 1.00 | 31.91  |
| ATOM | 603 | CA  | GLN | A | 79 | -9.743  | 42.334 | 69.829 | 1.00 | 30.53  |
| ATOM | 604 | C   | GLN | A | 79 | -8.425  | 42.981 | 70.197 | 1.00 | 34.86  |
| ATOM | 605 | O   | GLN | A | 79 | -7.340  | 42.497 | 69.903 | 1.00 | 33.78  |
| ATOM | 606 | CB  | GLN | A | 79 | -9.602  | 40.868 | 69.400 | 1.00 | 31.15  |
| ATOM | 607 | CG  | GLN | A | 79 | -10.980 | 40.241 | 69.104 | 1.00 | 35.70  |
| ATOM | 608 | CD  | GLN | A | 79 | -10.937 | 38.731 | 69.083 | 1.00 | 41.57  |
| ATOM | 609 | OE1 | GLN | A | 79 | -10.137 | 38.088 | 69.795 | 1.00 | 41.83  |
| ATOM | 610 | NE2 | GLN | A | 79 | -11.802 | 38.159 | 68.255 | 1.00 | 37.26  |
| ATOM | 611 | N   | SER | A | 80 | -8.566  | 44.149 | 70.795 | 1.00 | 28.82  |
| ATOM | 612 | CA  | SER | A | 80 | -7.443  | 44.951 | 71.184 | 1.00 | 25.23  |
| ATOM | 613 | C   | SER | A | 80 | -6.326  | 44.914 | 70.197 | 1.00 | 23.44  |
| ATOM | 614 | O   | SER | A | 80 | -6.479  | 45.361 | 69.076 | 1.00 | 26.59  |
| ATOM | 615 | CB  | SER | A | 80 | -6.889  | 44.746 | 72.585 | 1.00 | 31.25  |
| ATOM | 616 | OG  | SER | A | 80 | -6.560  | 43.393 | 72.744 | 1.00 | 36.44  |
| ATOM | 617 | N   | TYR | A | 81 | -5.174  | 44.420 | 70.668 | 1.00 | 20.57  |
| ATOM | 618 | CA  | TYR | A | 81 | -3.968  | 44.448 | 69.861 | 1.00 | 19.31  |
| ATOM | 619 | C   | TYR | A | 81 | -3.981  | 43.578 | 68.648 | 1.00 | 19.50  |
| ATOM | 620 | O   | TYR | A | 81 | -3.087  | 43.722 | 67.841 | 1.00 | 24.41  |
| ATOM | 621 | CB  | TYR | A | 81 | -2.638  | 44.225 | 70.624 | 1.00 | 20.60  |
| ATOM | 622 | CG  | TYR | A | 81 | -2.615  | 42.834 | 71.192 | 1.00 | 16.49  |
| ATOM | 623 | CD1 | TYR | A | 81 | -3.209  | 42.581 | 72.424 | 1.00 | 17.66  |
| ATOM | 624 | CD2 | TYR | A | 81 | -2.085  | 41.783 | 70.452 | 1.00 | 17.05  |



|      |     |     |     |   |    |         |        |        |      |       |
|------|-----|-----|-----|---|----|---------|--------|--------|------|-------|
| ATOM | 625 | CE1 | TYR | A | 81 | -3.258  | 41.294 | 72.944 | 1.00 | 20.70 |
| ATOM | 626 | CE2 | TYR | A | 81 | -2.178  | 40.481 | 70.933 | 1.00 | 18.17 |
| ATOM | 627 | CZ  | TYR | A | 81 | -2.731  | 40.249 | 72.192 | 1.00 | 21.91 |
| ATOM | 628 | OH  | TYR | A | 81 | -2.804  | 38.975 | 72.700 | 1.00 | 23.17 |
| ATOM | 629 | N   | LYS | A | 82 | -4.932  | 42.678 | 68.560 | 1.00 | 15.16 |
| ATOM | 630 | CA  | LYS | A | 82 | -5.023  | 41.797 | 67.414 | 1.00 | 16.93 |
| ATOM | 631 | C   | LYS | A | 82 | -5.794  | 42.437 | 66.270 | 1.00 | 29.18 |
| ATOM | 632 | O   | LYS | A | 82 | -5.780  | 41.883 | 65.177 | 1.00 | 28.33 |
| ATOM | 633 | CB  | LYS | A | 82 | -5.620  | 40.450 | 67.767 | 1.00 | 16.35 |
| ATOM | 634 | CG  | LYS | A | 82 | -5.110  | 39.966 | 69.106 | 1.00 | 32.81 |
| ATOM | 635 | CD  | LYS | A | 82 | -5.245  | 38.472 | 69.330 | 1.00 | 28.25 |
| ATOM | 636 | CE  | LYS | A | 82 | -5.699  | 38.100 | 70.734 | 1.00 | 39.59 |
| ATOM | 637 | NZ  | LYS | A | 82 | -6.304  | 36.762 | 70.827 | 1.00 | 41.62 |
| ATOM | 638 | N   | GLY | A | 83 | -6.437  | 43.596 | 66.510 | 1.00 | 24.43 |
| ATOM | 639 | CA  | GLY | A | 83 | -7.209  | 44.249 | 65.467 | 1.00 | 21.14 |
| ATOM | 640 | C   | GLY | A | 83 | -8.579  | 43.564 | 65.361 | 1.00 | 27.80 |
| ATOM | 641 | O   | GLY | A | 83 | -9.037  | 42.901 | 66.295 | 1.00 | 23.50 |
| ATOM | 642 | N   | SER | A | 84 | -9.218  | 43.674 | 64.186 | 1.00 | 28.99 |
| ATOM | 643 | CA  | SER | A | 84 | -10.541 | 43.072 | 63.948 | 1.00 | 27.81 |
| ATOM | 644 | C   | SER | A | 84 | -10.601 | 42.083 | 62.770 | 1.00 | 28.89 |
| ATOM | 645 | O   | SER | A | 84 | -10.153 | 42.340 | 61.646 | 1.00 | 27.83 |
| ATOM | 646 | CB  | SER | A | 84 | -11.619 | 44.136 | 63.732 | 1.00 | 30.17 |
| ATOM | 647 | OG  | SER | A | 84 | -11.229 | 45.402 | 64.258 | 1.00 | 40.66 |
| ATOM | 648 | N   | PRO | A | 85 | -11.210 | 40.949 | 63.053 | 1.00 | 22.21 |
| ATOM | 649 | CA  | PRO | A | 85 | -11.380 | 39.868 | 62.087 | 1.00 | 23.63 |
| ATOM | 650 | C   | PRO | A | 85 | -12.323 | 40.261 | 60.970 | 1.00 | 34.83 |
| ATOM | 651 | O   | PRO | A | 85 | -13.428 | 40.734 | 61.227 | 1.00 | 32.98 |
| ATOM | 652 | CB  | PRO | A | 85 | -12.094 | 38.750 | 62.838 | 1.00 | 20.66 |
| ATOM | 653 | CG  | PRO | A | 85 | -12.728 | 39.406 | 64.064 | 1.00 | 26.90 |
| ATOM | 654 | CD  | PRO | A | 85 | -12.026 | 40.748 | 64.281 | 1.00 | 19.24 |
| ATOM | 655 | N   | MET | A | 86 | -11.873 | 40.007 | 59.748 | 1.00 | 32.85 |
| ATOM | 656 | CA  | MET | A | 86 | -12.657 | 40.277 | 58.567 | 1.00 | 27.57 |
| ATOM | 657 | C   | MET | A | 86 | -13.107 | 38.999 | 57.876 | 1.00 | 35.20 |
| ATOM | 658 | O   | MET | A | 86 | -12.324 | 38.287 | 57.254 | 1.00 | 32.03 |
| ATOM | 659 | CB  | MET | A | 86 | -11.867 | 41.111 | 57.587 | 1.00 | 25.81 |
| ATOM | 660 | CG  | MET | A | 86 | -12.681 | 41.288 | 56.336 | 1.00 | 27.23 |
| ATOM | 661 | SD  | MET | A | 86 | -11.733 | 42.327 | 55.236 | 1.00 | 34.75 |
| ATOM | 662 | CE  | MET | A | 86 | -12.733 | 42.250 | 53.731 | 1.00 | 34.07 |
| ATOM | 663 | N   | GLU | A | 87 | -14.383 | 38.690 | 58.005 | 1.00 | 37.91 |
| ATOM | 664 | CA  | GLU | A | 87 | -14.920 | 37.509 | 57.352 | 1.00 | 37.56 |
| ATOM | 665 | C   | GLU | A | 87 | -15.419 | 37.749 | 55.916 | 1.00 | 38.67 |
| ATOM | 666 | O   | GLU | A | 87 | -16.161 | 38.678 | 55.590 | 1.00 | 35.07 |
| ATOM | 667 | CB  | GLU | A | 87 | -15.916 | 36.790 | 58.244 | 1.00 | 37.42 |
| ATOM | 668 | CG  | GLU | A | 87 | -16.428 | 35.494 |        |      |       |



|      |     |     |     |   |    |         |        |        |      |       |
|------|-----|-----|-----|---|----|---------|--------|--------|------|-------|
| ATOM | 683 | O   | SER | A | 89 | -17.690 | 35.614 | 49.475 | 1.00 | 42.76 |
| ATOM | 684 | CB  | SER | A | 89 | -19.556 | 35.586 | 51.839 | 1.00 | 50.73 |
| ATOM | 685 | OG  | SER | A | 89 | -19.993 | 35.504 | 53.187 | 1.00 | 74.19 |
| ATOM | 686 | N   | LEU | A | 90 | -17.458 | 33.462 | 50.220 | 1.00 | 40.59 |
| ATOM | 687 | CA  | LEU | A | 90 | -17.093 | 32.938 | 48.923 | 1.00 | 42.06 |
| ATOM | 688 | C   | LEU | A | 90 | -18.339 | 32.535 | 48.139 | 1.00 | 46.06 |
| ATOM | 689 | O   | LEU | A | 90 | -19.189 | 31.774 | 48.630 | 1.00 | 45.88 |
| ATOM | 690 | CB  | LEU | A | 90 | -16.141 | 31.743 | 49.082 | 1.00 | 42.14 |
| ATOM | 691 | CG  | LEU | A | 90 | -15.105 | 31.978 | 50.161 | 1.00 | 45.92 |
| ATOM | 692 | CD1 | LEU | A | 90 | -14.261 | 30.708 | 50.278 | 1.00 | 47.05 |
| ATOM | 693 | CD2 | LEU | A | 90 | -14.260 | 33.174 | 49.738 | 1.00 | 48.82 |
| ATOM | 694 | N   | PRO | A | 91 | -18.430 | 33.064 | 46.926 | 1.00 | 45.82 |
| ATOM | 695 | CA  | PRO | A | 91 | -19.562 | 32.786 | 46.048 | 1.00 | 49.29 |
| ATOM | 696 | C   | PRO | A | 91 | -19.576 | 31.355 | 45.482 | 1.00 | 56.99 |
| ATOM | 697 | O   | PRO | A | 91 | -20.552 | 30.965 | 44.859 | 1.00 | 55.61 |
| ATOM | 698 | CB  | PRO | A | 91 | -19.453 | 33.799 | 44.909 | 1.00 | 49.61 |
| ATOM | 699 | CG  | PRO | A | 91 | -18.042 | 34.369 | 44.955 | 1.00 | 53.03 |
| ATOM | 700 | CD  | PRO | A | 91 | -17.382 | 33.839 | 46.221 | 1.00 | 46.47 |
| ATOM | 701 | N   | ILE | A | 92 | -18.506 | 30.582 | 45.696 | 1.00 | 55.26 |
| ATOM | 702 | CA  | ILE | A | 92 | -18.422 | 29.211 | 45.223 | 1.00 | 58.60 |
| ATOM | 703 | C   | ILE | A | 92 | -17.760 | 28.334 | 46.273 | 1.00 | 58.73 |
| ATOM | 704 | O   | ILE | A | 92 | -16.685 | 28.673 | 46.724 | 1.00 | 61.40 |
| ATOM | 705 | CB  | ILE | A | 92 | -17.621 | 29.101 | 43.927 | 1.00 | 64.96 |
| ATOM | 706 | CG1 | ILE | A | 92 | -18.422 | 29.655 | 42.750 | 1.00 | 68.88 |
| ATOM | 707 | CG2 | ILE | A | 92 | -17.258 | 27.642 | 43.666 | 1.00 | 65.48 |
| ATOM | 708 | CD1 | ILE | A | 92 | -17.579 | 30.091 | 41.549 | 1.00 | 81.60 |
| ATOM | 709 | N   | ALA | A | 93 | -18.335 | 27.210 | 46.673 | 1.00 | 47.92 |
| ATOM | 710 | CA  | ALA | A | 93 | -17.613 | 26.441 | 47.657 | 1.00 | 44.97 |
| ATOM | 711 | C   | ALA | A | 93 | -16.291 | 26.029 | 47.044 | 1.00 | 53.08 |
| ATOM | 712 | O   | ALA | A | 93 | -16.279 | 25.772 | 45.841 | 1.00 | 54.26 |
| ATOM | 713 | CB  | ALA | A | 93 | -18.384 | 25.220 | 48.121 | 1.00 | 44.53 |
| ATOM | 714 | N   | LEU | A | 94 | -15.199 | 25.994 | 47.827 | 1.00 | 46.91 |
| ATOM | 715 | CA  | LEU | A | 94 | -13.894 | 25.607 | 47.304 | 1.00 | 43.41 |
| ATOM | 716 | C   | LEU | A | 94 | -13.570 | 24.240 | 47.797 | 1.00 | 46.24 |
| ATOM | 717 | O   | LEU | A | 94 | -14.042 | 23.826 | 48.851 | 1.00 | 47.66 |
| ATOM | 718 | CB  | LEU | A | 94 | -12.715 | 26.455 | 47.800 | 1.00 | 42.71 |
| ATOM | 719 | CG  | LEU | A | 94 | -12.601 | 27.799 | 47.109 | 1.00 | 48.37 |
| ATOM | 720 | CD1 | LEU | A | 94 | -11.307 | 28.510 | 47.507 | 1.00 | 45.33 |
| ATOM | 721 | CD2 | LEU | A | 94 | -12.659 | 27.584 | 45.600 | 1.00 | 57.15 |
| ATOM | 722 | N   | SER | A | 95 | -12.744 | 23.561 | 47.039 | 1.00 | 43.22 |
| ATOM | 723 | CA  | SER | A | 95 | -12.335 | 22.250 | 47.476 | 1.00 | 42.38 |
| ATOM | 724 | C   | SER | A | 95 | -10.834 | 22.238 | 47.628 | 1.00 | 36.34 |
| ATOM | 725 | O   | SER | A | 95 | -10.131 | 23.166 | 47.218 | 1.00 | 34.42 |
| ATOM | 726 | CB  | SER | A | 95 | -12.896 |        |        |      |       |



|      |     |     |     |   |     |         |        |        |      |        |
|------|-----|-----|-----|---|-----|---------|--------|--------|------|--------|
| ATOM | 741 | CB  | ASN | A | 97  | -5.257  | 21.772 | 45.817 | 1.00 | 29.05  |
| ATOM | 742 | CG  | ASN | A | 97  | -4.511  | 21.024 | 46.903 | 1.00 | 79.22  |
| ATOM | 743 | OD1 | ASN | A | 97  | -3.813  | 21.645 | 47.725 | 1.00 | 66.27  |
| ATOM | 744 | ND2 | ASN | A | 97  | -4.690  | 19.700 | 46.926 | 1.00 | 89.90  |
| ATOM | 745 | N   | GLN | A | 98  | -7.876  | 24.148 | 45.539 | 1.00 | 29.12  |
| ATOM | 746 | CA  | GLN | A | 98  | -8.480  | 25.068 | 44.628 | 1.00 | 30.69  |
| ATOM | 747 | C   | GLN | A | 98  | -8.245  | 26.455 | 45.151 | 1.00 | 34.12  |
| ATOM | 748 | O   | GLN | A | 98  | -8.220  | 26.673 | 46.363 | 1.00 | 32.27  |
| ATOM | 749 | CB  | GLN | A | 98  | -9.979  | 24.775 | 44.680 | 1.00 | 35.86  |
| ATOM | 750 | CG  | GLN | A | 98  | -10.299 | 23.404 | 44.057 | 1.00 | 52.64  |
| ATOM | 751 | CD  | GLN | A | 98  | -11.618 | 23.476 | 43.326 | 1.00 | 90.95  |
| ATOM | 752 | OE1 | GLN | A | 98  | -12.506 | 22.646 | 43.569 | 1.00 | 86.29  |
| ATOM | 753 | NE2 | GLN | A | 98  | -11.761 | 24.502 | 42.477 | 1.00 | 83.23  |
| ATOM | 754 | N   | GLU | A | 99  | -8.113  | 27.366 | 44.212 | 1.00 | 34.57  |
| ATOM | 755 | CA  | GLU | A | 99  | -7.836  | 28.767 | 44.459 | 1.00 | 35.24  |
| ATOM | 756 | C   | GLU | A | 99  | -8.799  | 29.788 | 43.877 | 1.00 | 42.30  |
| ATOM | 757 | O   | GLU | A | 99  | -9.240  | 29.696 | 42.731 | 1.00 | 42.60  |
| ATOM | 758 | CB  | GLU | A | 99  | -6.487  | 29.092 | 43.786 | 1.00 | 35.30  |
| ATOM | 759 | CG  | GLU | A | 99  | -5.592  | 27.856 | 43.665 | 1.00 | 43.60  |
| ATOM | 760 | CD  | GLU | A | 99  | -4.164  | 28.161 | 43.336 | 1.00 | 52.48  |
| ATOM | 761 | OE1 | GLU | A | 99  | -3.778  | 29.191 | 42.812 | 1.00 | 54.31  |
| ATOM | 762 | OE2 | GLU | A | 99  | -3.377  | 27.171 | 43.663 | 1.00 | 81.49  |
| ATOM | 763 | N   | ILE | A | 100 | -9.036  | 30.820 | 44.680 | 1.00 | 38.20  |
| ATOM | 764 | CA  | ILE | A | 100 | -9.820  | 31.975 | 44.306 | 1.00 | 37.64  |
| ATOM | 765 | C   | ILE | A | 100 | -8.939  | 33.193 | 44.501 | 1.00 | 47.53  |
| ATOM | 766 | O   | ILE | A | 100 | -7.889  | 33.202 | 45.153 | 1.00 | 46.12  |
| ATOM | 767 | CB  | ILE | A | 100 | -11.101 | 32.274 | 45.077 | 1.00 | 41.53  |
| ATOM | 768 | CG1 | ILE | A | 100 | -11.070 | 31.895 | 46.542 | 1.00 | 44.24  |
| ATOM | 769 | CG2 | ILE | A | 100 | -12.407 | 31.918 | 44.383 | 1.00 | 43.12  |
| ATOM | 770 | CD1 | ILE | A | 100 | -10.379 | 32.958 | 47.391 | 1.00 | 63.56  |
| ATOM | 771 | N   | VAL | A | 101 | -9.398  | 34.268 | 43.917 | 1.00 | 44.45  |
| ATOM | 772 | CA  | VAL | A | 101 | -8.706  | 35.510 | 44.086 | 1.00 | 41.52  |
| ATOM | 773 | C   | VAL | A | 101 | -9.710  | 36.529 | 44.565 | 1.00 | 44.93  |
| ATOM | 774 | O   | VAL | A | 101 | -10.794 | 36.664 | 44.001 | 1.00 | 43.66  |
| ATOM | 775 | CB  | VAL | A | 101 | -7.707  | 35.976 | 43.051 | 1.00 | 39.34  |
| ATOM | 776 | CG1 | VAL | A | 101 | -7.825  | 35.219 | 41.749 | 1.00 | 38.49  |
| ATOM | 777 | CG2 | VAL | A | 101 | -7.829  | 37.479 | 42.892 | 1.00 | 37.47  |
| ATOM | 778 | N   | ILE | A | 102 | -9.338  | 37.145 | 45.681 | 1.00 | 36.04  |
| ATOM | 779 | CA  | ILE | A | 102 | -10.137 | 38.122 | 46.378 | 1.00 | 30.61  |
| ATOM | 780 | C   | ILE | A | 102 | -9.440  | 39.463 | 46.313 | 1.00 | 33.94  |
| ATOM | 781 | O   | ILE | A | 102 | -8.294  | 39.614 | 46.776 | 1.00 | 33.48  |
| ATOM | 782 | CB  | ILE | A | 102 | -10.260 | 37.610 | 47.798 | 1.00 | 32.63  |
| ATOM | 783 | CG1 | ILE | A | 102 | -10.394 | 36.098 | 47.737 | 1.00 | 27.27  |
| ATOM | 784 | CG2 | ILE | A | 102 | -11.463 | 38.204 | 48.502 | 1.00 | 37.40  |
| ATOM | 785 | CD1 | ILE | A | 102 | -10.628 | 35.451 | 49.093 | 1.00 | 28.19  |
| ATOM | 786 | N   | GLU | A | 103 | -10.116 | 40.423 | 45.676 | 1.00 | 26.53  |
| ATOM | 787 | CA  | GLU | A | 103 | -9.549  | 41.755 | 45.548 | 1.00 | 27.13  |
| ATOM | 788 | C   | GLU | A | 103 | -10.186 | 42.615 | 46.601 | 1.00 | 37.89  |
| ATOM | 789 | O   | GLU | A | 103 | -11.408 | 42.630 | 46.710 | 1.00 | 40.69  |
| ATOM | 790 | CB  | GLU | A | 103 | -9.731  | 42.362 | 44.169 | 1.00 | 28.43  |
| ATOM | 791 | CG  | GLU | A | 103 | -8.946  | 43.670 | 44.000 | 1.00 | 39.11  |
| ATOM | 792 | CD  | GLU | A | 103 | -9.263  | 44.343 | 42.690 | 1.00 | 94.53  |
| ATOM | 793 | OE1 | GLU | A | 103 | -10.236 | 45.069 | 42.526 | 1.00 | 100.00 |
| ATOM | 794 | OE2 | GLU | A | 103 | -8.388  | 44.051 | 41.750 | 1.00 | 98.87  |
| ATOM | 795 | N   | ILE | A | 104 | -9.355  | 43.252 | 47.416 | 1.00 | 36.94  |
| ATOM | 796 | CA  | ILE | A | 104 | -9.847  | 44.076 | 48.512 | 1.00 | 35.20  |
| ATOM | 797 | C   | ILE | A | 104 | -9.459  | 45.532 | 48.378 | 1.00 | 38.03  |
| ATOM | 798 | O   | ILE | A | 104 | -8.277  | 45.856 | 48.192 | 1.00 | 34.77  |



|      |     |     |     |   |     |         |        |        |      |        |
|------|-----|-----|-----|---|-----|---------|--------|--------|------|--------|
| ATOM | 799 | CB  | ILE | A | 104 | -9.504  | 43.541 | 49.891 | 1.00 | 38.11  |
| ATOM | 800 | CG1 | ILE | A | 104 | -10.003 | 42.125 | 50.061 | 1.00 | 34.81  |
| ATOM | 801 | CG2 | ILE | A | 104 | -10.128 | 44.420 | 50.967 | 1.00 | 39.18  |
| ATOM | 802 | CD1 | ILE | A | 104 | -9.015  | 41.335 | 50.896 | 1.00 | 30.92  |
| ATOM | 803 | N   | SER | A | 105 | -10.529 | 46.353 | 48.429 | 1.00 | 42.46  |
| ATOM | 804 | CA  | SER | A | 105 | -10.510 | 47.811 | 48.323 | 1.00 | 42.36  |
| ATOM | 805 | C   | SER | A | 105 | -10.400 | 48.380 | 49.723 | 1.00 | 34.84  |
| ATOM | 806 | O   | SER | A | 105 | -11.328 | 48.305 | 50.510 | 1.00 | 31.47  |
| ATOM | 807 | CB  | SER | A | 105 | -11.731 | 48.328 | 47.575 | 1.00 | 45.94  |
| ATOM | 808 | OG  | SER | A | 105 | -11.386 | 48.517 | 46.209 | 1.00 | 47.45  |
| ATOM | 809 | N   | PHE | A | 106 | -9.228  | 48.910 | 50.031 | 1.00 | 33.13  |
| ATOM | 810 | CA  | PHE | A | 106 | -8.995  | 49.380 | 51.385 | 1.00 | 29.35  |
| ATOM | 811 | C   | PHE | A | 106 | -8.269  | 50.713 | 51.494 | 1.00 | 28.86  |
| ATOM | 812 | O   | PHE | A | 106 | -7.550  | 51.199 | 50.577 | 1.00 | 24.93  |
| ATOM | 813 | CB  | PHE | A | 106 | -8.134  | 48.290 | 52.115 | 1.00 | 27.98  |
| ATOM | 814 | CG  | PHE | A | 106 | -6.700  | 48.251 | 51.597 | 1.00 | 27.57  |
| ATOM | 815 | CD1 | PHE | A | 106 | -6.326  | 47.411 | 50.550 | 1.00 | 30.25  |
| ATOM | 816 | CD2 | PHE | A | 106 | -5.709  | 49.085 | 52.123 | 1.00 | 31.01  |
| ATOM | 817 | CE1 | PHE | A | 106 | -5.020  | 47.429 | 50.058 | 1.00 | 33.05  |
| ATOM | 818 | CE2 | PHE | A | 106 | -4.401  | 49.136 | 51.641 | 1.00 | 30.90  |
| ATOM | 819 | CZ  | PHE | A | 106 | -4.058  | 48.291 | 50.588 | 1.00 | 30.89  |
| ATOM | 820 | N   | GLU | A | 107 | -8.472  | 51.231 | 52.717 | 1.00 | 31.09  |
| ATOM | 821 | CA  | GLU | A | 107 | -7.864  | 52.476 | 53.183 | 1.00 | 36.36  |
| ATOM | 822 | C   | GLU | A | 107 | -7.271  | 52.257 | 54.583 | 1.00 | 33.60  |
| ATOM | 823 | O   | GLU | A | 107 | -7.945  | 51.706 | 55.468 | 1.00 | 34.10  |
| ATOM | 824 | CB  | GLU | A | 107 | -8.918  | 53.613 | 53.297 | 1.00 | 40.08  |
| ATOM | 825 | CG  | GLU | A | 107 | -8.512  | 55.003 | 52.740 | 1.00 | 64.89  |
| ATOM | 826 | CD  | GLU | A | 107 | -9.717  | 55.892 | 52.518 | 1.00 | 100.00 |
| ATOM | 827 | OE1 | GLU | A | 107 | -10.367 | 55.977 | 51.476 | 1.00 | 100.00 |
| ATOM | 828 | OE2 | GLU | A | 107 | -10.011 | 56.578 | 53.592 | 1.00 | 86.39  |
| ATOM | 829 | N   | THR | A | 108 | -6.019  | 52.681 | 54.788 | 1.00 | 32.30  |
| ATOM | 830 | CA  | THR | A | 108 | -5.408  | 52.538 | 56.114 | 1.00 | 35.58  |
| ATOM | 831 | C   | THR | A | 108 | -5.733  | 53.774 | 56.938 | 1.00 | 41.15  |
| ATOM | 832 | O   | THR | A | 108 | -6.045  | 54.814 | 56.360 | 1.00 | 39.58  |
| ATOM | 833 | CB  | THR | A | 108 | -3.864  | 52.454 | 56.088 | 1.00 | 36.81  |
| ATOM | 834 | OG1 | THR | A | 108 | -3.268  | 53.544 | 55.381 | 1.00 | 33.05  |
| ATOM | 835 | CG2 | THR | A | 108 | -3.418  | 51.100 | 55.560 | 1.00 | 27.41  |
| ATOM | 836 | N   | SER | A | 109 | -5.608  | 53.647 | 58.258 | 1.00 | 34.04  |
| ATOM | 837 | CA  | SER | A | 109 | -5.823  | 54.723 | 59.207 | 1.00 | 27.85  |
| ATOM | 838 | C   | SER | A | 109 | -4.559  | 55.540 | 59.361 | 1.00 | 33.11  |
| ATOM | 839 | O   | SER | A | 109 | -3.447  | 55.011 | 59.228 | 1.00 | 29.81  |
| ATOM | 840 | CB  | SER | A | 109 | -6.278  | 54.179 | 60.541 | 1.00 | 26.33  |
| ATOM | 841 | OG  | SER | A | 109 | -6.058  | 55.183 | 61.512 | 1.00 | 36.95  |
| ATOM | 842 | N   | PRO | A | 1   |         |        |        |      |        |



009220 DT22109

|      |     |     |     |   |     |        |        |        |            |
|------|-----|-----|-----|---|-----|--------|--------|--------|------------|
| ATOM | 857 | NZ  | LYS | A | 111 | -7.898 | 58.618 | 64.591 | 1.00100.00 |
| ATOM | 858 | N   | SER | A | 112 | -2.237 | 54.000 | 61.775 | 1.00 25.30 |
| ATOM | 859 | CA  | SER | A | 112 | -1.816 | 52.609 | 61.553 | 1.00 22.00 |
| ATOM | 860 | C   | SER | A | 112 | -0.545 | 52.268 | 62.367 | 1.00 19.89 |
| ATOM | 861 | O   | SER | A | 112 | 0.496  | 52.894 | 62.223 | 1.00 23.91 |
| ATOM | 862 | CB  | SER | A | 112 | -1.541 | 52.354 | 60.072 | 1.00 15.83 |
| ATOM | 863 | OG  | SER | A | 112 | -0.793 | 51.153 | 59.917 | 1.00 19.70 |
| ATOM | 864 | N   | SER | A | 113 | -0.613 | 51.245 | 63.195 | 1.00 18.58 |
| ATOM | 865 | CA  | SER | A | 113 | 0.525  | 50.842 | 64.006 | 1.00 18.61 |
| ATOM | 866 | C   | SER | A | 113 | 1.734  | 50.356 | 63.211 | 1.00 24.91 |
| ATOM | 867 | O   | SER | A | 113 | 2.859  | 50.239 | 63.718 | 1.00 22.90 |
| ATOM | 868 | CB  | SER | A | 113 | 0.114  | 49.900 | 65.120 | 1.00 19.15 |
| ATOM | 869 | OG  | SER | A | 113 | -0.312 | 48.649 | 64.620 | 1.00 19.49 |
| ATOM | 870 | N   | ALA | A | 114 | 1.499  | 50.077 | 61.937 | 1.00 19.34 |
| ATOM | 871 | CA  | ALA | A | 114 | 2.541  | 49.589 | 61.053 | 1.00 17.80 |
| ATOM | 872 | C   | ALA | A | 114 | 3.310  | 50.728 | 60.449 | 1.00 20.40 |
| ATOM | 873 | O   | ALA | A | 114 | 4.371  | 50.555 | 59.817 | 1.00 19.02 |
| ATOM | 874 | CB  | ALA | A | 114 | 1.850  | 48.892 | 59.883 | 1.00 16.86 |
| ATOM | 875 | N   | LEU | A | 115 | 2.724  | 51.914 | 60.607 | 1.00 17.74 |
| ATOM | 876 | CA  | LEU | A | 115 | 3.358  | 53.026 | 59.960 | 1.00 19.94 |
| ATOM | 877 | C   | LEU | A | 115 | 3.643  | 54.215 | 60.826 | 1.00 19.68 |
| ATOM | 878 | O   | LEU | A | 115 | 3.052  | 54.427 | 61.870 | 1.00 24.55 |
| ATOM | 879 | CB  | LEU | A | 115 | 2.440  | 53.538 | 58.829 | 1.00 22.23 |
| ATOM | 880 | CG  | LEU | A | 115 | 1.963  | 52.455 | 57.873 | 1.00 25.61 |
| ATOM | 881 | CD1 | LEU | A | 115 | 0.865  | 53.050 | 57.001 | 1.00 29.64 |
| ATOM | 882 | CD2 | LEU | A | 115 | 3.101  | 51.926 | 56.999 | 1.00 20.12 |
| ATOM | 883 | N   | GLN | A | 116 | 4.578  | 54.971 | 60.308 | 1.00 18.97 |
| ATOM | 884 | CA  | GLN | A | 116 | 4.990  | 56.249 | 60.865 | 1.00 22.74 |
| ATOM | 885 | C   | GLN | A | 116 | 5.083  | 57.265 | 59.739 | 1.00 24.89 |
| ATOM | 886 | O   | GLN | A | 116 | 5.911  | 57.131 | 58.823 | 1.00 20.48 |
| ATOM | 887 | CB  | GLN | A | 116 | 6.265  | 56.308 | 61.706 | 1.00 23.66 |
| ATOM | 888 | CG  | GLN | A | 116 | 6.278  | 57.643 | 62.492 | 1.00 31.55 |
| ATOM | 889 | CD  | GLN | A | 116 | 7.541  | 57.860 | 63.291 | 1.00 28.17 |
| ATOM | 890 | OE1 | GLN | A | 116 | 8.409  | 56.973 | 63.387 | 1.00 23.94 |
| ATOM | 891 | NE2 | GLN | A | 116 | 7.681  | 59.062 | 63.834 | 1.00 24.04 |
| ATOM | 892 | N   | TRP | A | 117 | 4.202  | 58.261 | 59.817 | 1.00 25.51 |
| ATOM | 893 | CA  | TRP | A | 117 | 4.154  | 59.323 | 58.829 | 1.00 24.50 |
| ATOM | 894 | C   | TRP | A | 117 | 4.873  | 60.524 | 59.411 | 1.00 29.40 |
| ATOM | 895 | O   | TRP | A | 117 | 4.437  | 61.044 | 60.438 | 1.00 32.14 |
| ATOM | 896 | CB  | TRP | A | 117 | 2.697  | 59.715 | 58.631 | 1.00 22.31 |
| ATOM | 897 | CG  | TRP | A | 117 | 1.865  | 58.712 | 57.898 | 1.00 24.18 |
| ATOM | 898 | CD1 | TRP | A | 117 | 1.075  | 57.767 | 58.475 | 1.00 27.24 |
| ATOM | 899 | CD2 | TRP | A | 117 | 1.671  | 58.606 | 56.469 | 1.00 23.00 |
| ATOM | 900 | NE1 | TRP | A | 117 | 0.429  | 57.046 | 57.492 | 1.00 26.67 |
| ATOM | 901 | CE2 | TRP | A | 117 | 0.772  | 57.531 | 56.253 | 1.00 26.59 |
| ATOM | 902 | CE3 | TRP | A | 117 | 2.185  | 59.296 | 55.364 | 1.00 24.86 |
| ATOM | 903 | CZ2 | TRP | A | 117 | 0.347  | 57.145 | 54.973 | 1.00 25.38 |
| ATOM | 904 | CZ3 | TRP | A | 117 | 1.789  | 58.900 | 54.090 | 1.00 27.68 |
| ATOM | 905 | CH2 | TRP | A | 117 | 0.868  | 57.855 | 53.901 | 1.00 28.07 |
| ATOM | 906 | N   | LEU | A | 118 | 5.972  | 60.918 | 58.769 | 1.00 23.97 |
| ATOM | 907 | CA  | LEU | A | 118 | 6.813  | 62.038 | 59.185 | 1.00 25.88 |
| ATOM | 908 | C   | LEU | A | 118 | 6.557  | 63.335 | 58.404 | 1.00 35.42 |
| ATOM | 909 | O   | LEU | A | 118 | 6.471  | 63.345 | 57.171 | 1.00 37.58 |
| ATOM | 910 | CB  | LEU | A | 118 | 8.346  | 61.756 | 59.042 | 1.00 24.73 |
| ATOM | 911 | CG  | LEU | A | 118 | 8.904  | 60.441 | 59.630 | 1.00 31.22 |
| ATOM | 912 | CD1 | LEU | A | 118 | 10.425 | 60.511 | 59.713 | 1.00 27.63 |
| ATOM | 913 | CD2 | LEU | A | 118 | 8.372  | 60.198 | 61.033 | 1.00 35.89 |
| ATOM | 914 | N   | THR | A | 119 | 6.493  | 64.452 | 59.136 | 1.00 29.43 |



|      |     |     |     |   |     |        |        |        |      |        |
|------|-----|-----|-----|---|-----|--------|--------|--------|------|--------|
| ATOM | 915 | CA  | THR | A | 119 | 6.345  | 65.763 | 58.528 | 1.00 | 26.58  |
| ATOM | 916 | C   | THR | A | 119 | 7.723  | 66.117 | 58.011 | 1.00 | 28.74  |
| ATOM | 917 | O   | THR | A | 119 | 8.715  | 65.587 | 58.515 | 1.00 | 33.10  |
| ATOM | 918 | CB  | THR | A | 119 | 5.913  | 66.773 | 59.610 | 1.00 | 30.87  |
| ATOM | 919 | OG1 | THR | A | 119 | 6.959  | 66.918 | 60.570 | 1.00 | 43.03  |
| ATOM | 920 | CG2 | THR | A | 119 | 4.662  | 66.239 | 60.288 | 1.00 | 35.04  |
| ATOM | 921 | N   | PRO | A | 120 | 7.833  | 67.008 | 57.023 | 1.00 | 30.76  |
| ATOM | 922 | CA  | PRO | A | 120 | 9.151  | 67.332 | 56.511 | 1.00 | 27.85  |
| ATOM | 923 | C   | PRO | A | 120 | 10.131 | 67.791 | 57.577 | 1.00 | 33.68  |
| ATOM | 924 | O   | PRO | A | 120 | 11.342 | 67.593 | 57.442 | 1.00 | 34.58  |
| ATOM | 925 | CB  | PRO | A | 120 | 8.944  | 68.390 | 55.431 | 1.00 | 29.01  |
| ATOM | 926 | CG  | PRO | A | 120 | 7.483  | 68.312 | 55.046 | 1.00 | 29.59  |
| ATOM | 927 | CD  | PRO | A | 120 | 6.768  | 67.680 | 56.215 | 1.00 | 27.06  |
| ATOM | 928 | N   | GLU | A | 121 | 9.603  | 68.413 | 58.628 | 1.00 | 36.28  |
| ATOM | 929 | CA  | GLU | A | 121 | 10.428 | 68.913 | 59.735 | 1.00 | 41.71  |
| ATOM | 930 | C   | GLU | A | 121 | 11.155 | 67.780 | 60.421 | 1.00 | 46.90  |
| ATOM | 931 | O   | GLU | A | 121 | 12.302 | 67.911 | 60.852 | 1.00 | 45.40  |
| ATOM | 932 | CB  | GLU | A | 121 | 9.653  | 69.674 | 60.828 | 1.00 | 43.86  |
| ATOM | 933 | CG  | GLU | A | 121 | 8.117  | 69.533 | 60.744 | 1.00 | 58.00  |
| ATOM | 934 | CD  | GLU | A | 121 | 7.497  | 70.524 | 59.787 | 1.00 | 95.29  |
| ATOM | 935 | OE1 | GLU | A | 121 | 8.029  | 71.583 | 59.481 | 1.00 | 100.00 |
| ATOM | 936 | OE2 | GLU | A | 121 | 6.343  | 70.133 | 59.295 | 1.00 | 59.19  |
| ATOM | 937 | N   | GLN | A | 122 | 10.419 | 66.674 | 60.509 | 1.00 | 40.04  |
| ATOM | 938 | CA  | GLN | A | 122 | 10.898 | 65.442 | 61.105 | 1.00 | 34.75  |
| ATOM | 939 | C   | GLN | A | 122 | 11.970 | 64.761 | 60.246 | 1.00 | 38.46  |
| ATOM | 940 | O   | GLN | A | 122 | 12.575 | 63.775 | 60.657 | 1.00 | 36.92  |
| ATOM | 941 | CB  | GLN | A | 122 | 9.688  | 64.505 | 61.280 | 1.00 | 31.67  |
| ATOM | 942 | CG  | GLN | A | 122 | 9.002  | 64.705 | 62.627 | 1.00 | 23.93  |
| ATOM | 943 | CD  | GLN | A | 122 | 7.722  | 63.930 | 62.790 | 1.00 | 33.52  |
| ATOM | 944 | OE1 | GLN | A | 122 | 6.754  | 64.126 | 62.036 | 1.00 | 38.04  |
| ATOM | 945 | NE2 | GLN | A | 122 | 7.682  | 63.071 | 63.806 | 1.00 | 30.07  |
| ATOM | 946 | N   | THR | A | 123 | 12.202 | 65.252 | 59.018 | 1.00 | 36.12  |
| ATOM | 947 | CA  | THR | A | 123 | 13.166 | 64.626 | 58.102 | 1.00 | 33.51  |
| ATOM | 948 | C   | THR | A | 123 | 14.492 | 65.315 | 58.131 | 1.00 | 36.18  |
| ATOM | 949 | O   | THR | A | 123 | 14.617 | 66.359 | 58.755 | 1.00 | 40.90  |
| ATOM | 950 | CB  | THR | A | 123 | 12.671 | 64.577 | 56.637 | 1.00 | 31.27  |
| ATOM | 951 | OG1 | THR | A | 123 | 12.565 | 65.900 | 56.137 | 1.00 | 38.36  |
| ATOM | 952 | CG2 | THR | A | 123 | 11.300 | 63.912 | 56.566 | 1.00 | 21.97  |
| ATOM | 953 | N   | SER | A | 124 | 15.470 | 64.743 | 57.448 | 1.00 | 30.18  |
| ATOM | 954 | CA  | SER | A | 124 | 16.767 | 65.373 | 57.441 | 1.00 | 30.34  |
| ATOM | 955 | C   | SER | A | 124 | 16.774 | 66.616 | 56.579 | 1.00 | 39.98  |
| ATOM | 956 | O   | SER | A | 124 | 17.434 | 67.609 | 56.904 | 1.00 | 42.72  |
| ATOM | 957 | CB  | SER | A | 124 | 17.881 | 64.484 | 56.905 | 1.00 | 31.00  |
| ATOM | 958 | OG  | SER | A | 124 | 18.222 | 63.434 | 57.794 | 1.00 | 41.86  |
| ATOM | 959 | N   | GLY | A | 125 | 16.061 | 66.515 | 55.460 | 1.00 | 33.12  |
| ATOM | 960 | CA  | GLY | A | 125 | 16.018 | 67.566 | 54.465 | 1.00 | 33.55  |
| ATOM | 961 | C   | GLY | A | 125 | 15.115 | 68.725 | 54.777 | 1.00 | 39.54  |
| ATOM | 962 | O   | GLY | A | 125 | 15.324 | 69.828 | 54.271 | 1.00 | 43.14  |
| ATOM | 963 | N   | LYS | A | 126 | 14.105 | 68.443 | 55.574 | 1.00 | 34.88  |
| ATOM | 964 | CA  | LYS | A | 126 | 13.198 | 69.487 | 55.950 | 1.00 | 35.05  |
| ATOM | 965 | C   | LYS | A | 126 | 12.225 | 69.949 | 54.863 | 1.00 | 43.18  |
| ATOM | 966 | O   | LYS | A | 126 | 11.309 | 70.745 | 55.156 | 1.00 | 41.50  |
| ATOM | 967 | CB  | LYS | A | 126 | 13.976 | 70.652 | 56.539 | 1.00 | 34.53  |
| ATOM | 968 | CG  | LYS | A | 126 | 15.059 | 70.188 | 57.493 | 1.00 | 33.17  |
| ATOM | 969 | CD  | LYS | A | 126 | 14.496 | 69.475 | 58.710 | 1.00 | 28.58  |
| ATOM | 970 | CE  | LYS | A | 126 | 15.597 | 69.005 | 59.656 | 1.00 | 35.70  |
| ATOM | 971 | NZ  | LYS | A | 126 | 15.099 | 68.062 | 60.666 | 1.00 | 53.76  |
| ATOM | 972 | N   | GLU | A | 127 | 12.397 | 69.456 | 53.632 | 1.00 | 34.06  |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 973  | CA  | GLU | A | 127 | 11.497 | 69.879 | 52.579 | 1.00 | 32.35 |
| ATOM | 974  | C   | GLU | A | 127 | 10.481 | 68.870 | 52.125 | 1.00 | 41.06 |
| ATOM | 975  | O   | GLU | A | 127 | 9.583  | 69.214 | 51.369 | 1.00 | 41.24 |
| ATOM | 976  | CB  | GLU | A | 127 | 12.231 | 70.396 | 51.348 | 1.00 | 32.73 |
| ATOM | 977  | CG  | GLU | A | 127 | 13.167 | 71.542 | 51.745 | 1.00 | 41.87 |
| ATOM | 978  | CD  | GLU | A | 127 | 12.515 | 72.883 | 51.595 | 1.00 | 68.20 |
| ATOM | 979  | OE1 | GLU | A | 127 | 11.668 | 73.152 | 50.750 | 1.00 | 85.44 |
| ATOM | 980  | OE2 | GLU | A | 127 | 13.008 | 73.747 | 52.442 | 1.00 | 94.35 |
| ATOM | 981  | N   | HIS | A | 128 | 10.603 | 67.636 | 52.556 | 1.00 | 38.36 |
| ATOM | 982  | CA  | HIS | A | 128 | 9.649  | 66.635 | 52.130 | 1.00 | 36.38 |
| ATOM | 983  | C   | HIS | A | 128 | 9.272  | 65.683 | 53.241 | 1.00 | 34.84 |
| ATOM | 984  | O   | HIS | A | 128 | 10.054 | 65.414 | 54.148 | 1.00 | 33.92 |
| ATOM | 985  | CB  | HIS | A | 128 | 10.311 | 65.761 | 51.062 | 1.00 | 39.67 |
| ATOM | 986  | CG  | HIS | A | 128 | 10.775 | 66.438 | 49.801 | 1.00 | 44.07 |
| ATOM | 987  | ND1 | HIS | A | 128 | 9.885  | 66.842 | 48.810 | 1.00 | 44.77 |
| ATOM | 988  | CD2 | HIS | A | 128 | 12.031 | 66.713 | 49.378 | 1.00 | 44.57 |
| ATOM | 989  | CE1 | HIS | A | 128 | 10.611 | 67.349 | 47.836 | 1.00 | 44.22 |
| ATOM | 990  | NE2 | HIS | A | 128 | 11.905 | 67.291 | 48.144 | 1.00 | 44.43 |
| ATOM | 991  | N   | PRO | A | 129 | 8.084  | 65.124 | 53.134 | 1.00 | 30.93 |
| ATOM | 992  | CA  | PRO | A | 129 | 7.662  | 64.165 | 54.115 | 1.00 | 30.73 |
| ATOM | 993  | C   | PRO | A | 129 | 8.383  | 62.819 | 53.902 | 1.00 | 32.60 |
| ATOM | 994  | O   | PRO | A | 129 | 9.307  | 62.688 | 53.088 | 1.00 | 30.87 |
| ATOM | 995  | CB  | PRO | A | 129 | 6.152  | 64.031 | 53.955 | 1.00 | 28.47 |
| ATOM | 996  | CG  | PRO | A | 129 | 5.892  | 64.328 | 52.506 | 1.00 | 28.59 |
| ATOM | 997  | CD  | PRO | A | 129 | 7.023  | 65.264 | 52.115 | 1.00 | 29.83 |
| ATOM | 998  | N   | TYR | A | 130 | 7.991  | 61.816 | 54.680 | 1.00 | 24.05 |
| ATOM | 999  | CA  | TYR | A | 130 | 8.641  | 60.521 | 54.581 | 1.00 | 23.32 |
| ATOM | 1000 | C   | TYR | A | 130 | 7.739  | 59.482 | 55.193 | 1.00 | 27.11 |
| ATOM | 1001 | O   | TYR | A | 130 | 7.054  | 59.735 | 56.169 | 1.00 | 25.99 |
| ATOM | 1002 | CB  | TYR | A | 130 | 9.927  | 60.574 | 55.425 | 1.00 | 24.39 |
| ATOM | 1003 | CG  | TYR | A | 130 | 10.932 | 59.447 | 55.270 | 1.00 | 26.41 |
| ATOM | 1004 | CD1 | TYR | A | 130 | 10.681 | 58.134 | 55.683 | 1.00 | 26.44 |
| ATOM | 1005 | CD2 | TYR | A | 130 | 12.195 | 59.750 | 54.765 | 1.00 | 26.16 |
| ATOM | 1006 | CE1 | TYR | A | 130 | 11.650 | 57.136 | 55.575 | 1.00 | 19.38 |
| ATOM | 1007 | CE2 | TYR | A | 130 | 13.179 | 58.768 | 54.644 | 1.00 | 26.74 |
| ATOM | 1008 | CZ  | TYR | A | 130 | 12.900 | 57.463 | 55.047 | 1.00 | 21.41 |
| ATOM | 1009 | OH  | TYR | A | 130 | 13.904 | 56.550 | 54.915 | 1.00 | 24.90 |
| ATOM | 1010 | N   | LEU | A | 131 | 7.704  | 58.299 | 54.639 | 1.00 | 26.48 |
| ATOM | 1011 | CA  | LEU | A | 131 | 6.846  | 57.288 | 55.247 | 1.00 | 26.34 |
| ATOM | 1012 | C   | LEU | A | 131 | 7.626  | 55.976 | 55.315 | 1.00 | 29.76 |
| ATOM | 1013 | O   | LEU | A | 131 | 8.394  | 55.705 | 54.383 | 1.00 | 30.08 |
| ATOM | 1014 | CB  | LEU | A | 131 | 5.511  | 57.120 | 54.477 | 1.00 | 24.01 |
| ATOM | 1015 | CG  | LEU | A | 131 | 4.873  | 55.750 | 54.658 | 1.00 | 25.25 |
| ATOM | 1016 | CD1 | LEU | A | 131 | 3.923  | 55.774 | 55.850 | 1.00 | 22.47 |
| ATOM | 1017 | CD2 | LEU | A | 131 | 4.091  | 55.343 | 53.420 | 1.00 | 26.97 |
| ATOM | 1018 | N   | PHE | A | 132 | 7.467  | 55.207 | 56.412 | 1.00 | 24.85 |
| ATOM | 1019 | CA  | PHE | A | 132 | 8.122  | 53.906 | 56.569 | 1.00 | 22.86 |
| ATOM | 1020 | C   | PHE | A | 132 | 7.245  | 52.905 | 57.318 | 1.00 | 23.01 |
| ATOM | 1021 | O   | PHE | A | 132 | 6.475  | 53.255 | 58.209 | 1.00 | 20.93 |
| ATOM | 1022 | CB  | PHE | A | 132 | 9.575  | 53.929 | 57.083 | 1.00 | 26.88 |
| ATOM | 1023 | CG  | PHE | A | 132 | 9.667  | 54.245 | 58.567 | 1.00 | 29.09 |
| ATOM | 1024 | CD1 | PHE | A | 132 | 9.345  | 53.286 | 59.532 | 1.00 | 28.26 |
| ATOM | 1025 | CD2 | PHE | A | 132 | 10.052 | 55.514 | 59.005 | 1.00 | 29.01 |
| ATOM | 1026 | CE1 | PHE | A | 132 | 9.422  | 53.564 | 60.899 | 1.00 | 23.76 |
| ATOM | 1027 | CE2 | PHE | A | 132 | 10.124 | 55.822 | 60.364 | 1.00 | 26.04 |
| ATOM | 1028 | CZ  | PHE | A | 132 | 9.808  | 54.842 | 61.304 | 1.00 | 20.79 |
| ATOM | 1029 | N   | SER | A | 133 | 7.319  | 51.632 | 56.959 | 1.00 | 20.01 |
| ATOM | 1030 | CA  | SER | A | 133 | 6.487  | 50.644 | 57.614 | 1.00 | 18.49 |



|      |      |     |           |        |        |        |      |       |
|------|------|-----|-----------|--------|--------|--------|------|-------|
| ATOM | 1031 | C   | SER A 133 | 7.343  | 49.758 | 58.499 | 1.00 | 20.07 |
| ATOM | 1032 | O   | SER A 133 | 8.565  | 49.721 | 58.408 | 1.00 | 20.93 |
| ATOM | 1033 | CB  | SER A 133 | 5.820  | 49.721 | 56.600 | 1.00 | 21.00 |
| ATOM | 1034 | OG  | SER A 133 | 6.794  | 48.889 | 55.979 | 1.00 | 19.33 |
| ATOM | 1035 | N   | GLN A 134 | 6.652  | 49.019 | 59.349 | 1.00 | 17.53 |
| ATOM | 1036 | CA  | GLN A 134 | 7.307  | 48.078 | 60.224 | 1.00 | 16.15 |
| ATOM | 1037 | C   | GLN A 134 | 6.253  | 47.039 | 60.602 | 1.00 | 21.22 |
| ATOM | 1038 | O   | GLN A 134 | 5.445  | 47.228 | 61.500 | 1.00 | 20.50 |
| ATOM | 1039 | CB  | GLN A 134 | 8.094  | 48.787 | 61.354 | 1.00 | 15.03 |
| ATOM | 1040 | CG  | GLN A 134 | 8.497  | 47.798 | 62.475 | 1.00 | 22.80 |
| ATOM | 1041 | CD  | GLN A 134 | 9.449  | 46.740 | 61.953 | 1.00 | 32.47 |
| ATOM | 1042 | OE1 | GLN A 134 | 10.430 | 47.087 | 61.278 | 1.00 | 20.01 |
| ATOM | 1043 | NE2 | GLN A 134 | 9.174  | 45.470 | 62.246 | 1.00 | 18.65 |
| ATOM | 1044 | N   | CYS A 135 | 6.173  | 45.933 | 59.853 | 1.00 | 20.27 |
| ATOM | 1045 | CA  | CYS A 135 | 5.121  | 44.948 | 60.131 | 1.00 | 19.65 |
| ATOM | 1046 | C   | CYS A 135 | 5.386  | 43.913 | 61.204 | 1.00 | 19.96 |
| ATOM | 1047 | O   | CYS A 135 | 4.454  | 43.422 | 61.822 | 1.00 | 16.67 |
| ATOM | 1048 | CB  | CYS A 135 | 4.662  | 44.209 | 58.847 | 1.00 | 18.98 |
| ATOM | 1049 | SG  | CYS A 135 | 4.157  | 45.396 | 57.599 | 1.00 | 22.04 |
| ATOM | 1050 | N   | GLN A 136 | 6.646  | 43.517 | 61.379 | 1.00 | 20.85 |
| ATOM | 1051 | CA  | GLN A 136 | 6.936  | 42.489 | 62.366 | 1.00 | 19.49 |
| ATOM | 1052 | C   | GLN A 136 | 6.654  | 43.049 | 63.750 | 1.00 | 17.79 |
| ATOM | 1053 | O   | GLN A 136 | 7.052  | 44.180 | 64.026 | 1.00 | 19.64 |
| ATOM | 1054 | CB  | GLN A 136 | 8.388  | 41.945 | 62.208 | 1.00 | 18.24 |
| ATOM | 1055 | CG  | GLN A 136 | 8.670  | 40.708 | 63.090 | 1.00 | 15.69 |
| ATOM | 1056 | CD  | GLN A 136 | 10.104 | 40.218 | 62.989 | 1.00 | 18.82 |
| ATOM | 1057 | OE1 | GLN A 136 | 10.987 | 40.986 | 62.591 | 1.00 | 21.40 |
| ATOM | 1058 | NE2 | GLN A 136 | 10.344 | 38.964 | 63.370 | 1.00 | 20.32 |
| ATOM | 1059 | N   | ALA A 137 | 5.965  | 42.280 | 64.605 | 1.00 | 16.00 |
| ATOM | 1060 | CA  | ALA A 137 | 5.459  | 40.921 | 64.361 | 1.00 | 13.64 |
| ATOM | 1061 | C   | ALA A 137 | 4.096  | 40.891 | 63.680 | 1.00 | 20.13 |
| ATOM | 1062 | O   | ALA A 137 | 3.915  | 40.228 | 62.670 | 1.00 | 19.24 |
| ATOM | 1063 | CB  | ALA A 137 | 5.345  | 40.115 | 65.651 | 1.00 | 13.33 |
| ATOM | 1064 | N   | ILE A 138 | 3.130  | 41.599 | 64.237 | 1.00 | 17.65 |
| ATOM | 1065 | CA  | ILE A 138 | 1.812  | 41.538 | 63.646 | 1.00 | 17.65 |
| ATOM | 1066 | C   | ILE A 138 | 1.182  | 42.859 | 63.250 | 1.00 | 17.89 |
| ATOM | 1067 | O   | ILE A 138 | 0.080  | 43.166 | 63.648 | 1.00 | 18.12 |
| ATOM | 1068 | CB  | ILE A 138 | 0.905  | 40.782 | 64.584 | 1.00 | 21.50 |
| ATOM | 1069 | CG1 | ILE A 138 | 0.909  | 41.474 | 65.949 | 1.00 | 23.03 |
| ATOM | 1070 | CG2 | ILE A 138 | 1.365  | 39.325 | 64.715 | 1.00 | 17.85 |
| ATOM | 1071 | CD1 | ILE A 138 | -0.197 | 40.954 | 66.864 | 1.00 | 20.51 |
| ATOM | 1072 | N   | HIS A 139 | 1.883  | 43.639 | 62.477 | 1.00 | 14.35 |
| ATOM | 1073 | CA  | HIS A 139 | 1.347  | 44.918 | 62.069 | 1.00 | 20.04 |
| ATOM | 1074 | C   | HIS A 139 | 0.947  | 44.960 | 60.586 | 1.00 | 22.63 |
| ATOM | 1075 | O   | HIS A 139 | 0.405  | 45.970 | 60.153 | 1.00 | 21.50 |
| ATOM | 1076 | CB  | HIS A 139 | 2.294  | 46.104 | 62.418 | 1.00 | 20.69 |
| ATOM | 1077 | CG  | HIS A 139 | 2.542  | 46.181 | 63.905 | 1.00 | 22.28 |
| ATOM | 1078 | ND1 | HIS A 139 | 1.598  | 46.682 | 64.780 | 1.00 | 21.42 |
| ATOM | 1079 | CD2 | HIS A 139 | 3.607  | 45.772 | 64.641 | 1.00 | 20.30 |
| ATOM | 1080 | CE1 | HIS A 139 | 2.102  | 46.574 | 66.004 | 1.00 | 21.50 |
| ATOM | 1081 | NE2 | HIS A 139 | 3.316  | 46.043 | 65.948 | 1.00 | 20.79 |
| ATOM | 1082 | N   | CYS A 140 | 1.231  | 43.891 | 59.817 | 1.00 | 23.70 |
| ATOM | 1083 | CA  | CYS A 140 | 0.854  | 43.842 | 58.393 | 1.00 | 20.51 |
| ATOM | 1084 | C   | CYS A 140 | -0.641 | 44.154 | 58.238 | 1.00 | 18.21 |
| ATOM | 1085 | O   | CYS A 140 | -1.080 | 44.926 | 57.384 | 1.00 | 21.51 |
| ATOM | 1086 | CB  | CYS A 140 | 1.244  | 42.523 | 57.676 | 1.00 | 18.69 |
| ATOM | 1087 | SG  | CYS A 140 | 1.220  | 42.744 | 55.865 | 1.00 | 23.45 |
| ATOM | 1088 | N   | ARG A 141 | -1.403 | 43.548 | 59.139 | 1.00 | 17.49 |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 1089 | CA  | ARG | A | 141 | -2.849 | 43.681 | 59.236 | 1.00 | 19.29 |
| ATOM | 1090 | C   | ARG | A | 141 | -3.305 | 45.119 | 59.365 | 1.00 | 29.79 |
| ATOM | 1091 | O   | ARG | A | 141 | -4.507 | 45.415 | 59.189 | 1.00 | 29.48 |
| ATOM | 1092 | CB  | ARG | A | 141 | -3.435 | 42.857 | 60.368 | 1.00 | 19.28 |
| ATOM | 1093 | CG  | ARG | A | 141 | -3.041 | 43.331 | 61.779 | 1.00 | 17.77 |
| ATOM | 1094 | CD  | ARG | A | 141 | -3.499 | 42.358 | 62.853 | 1.00 | 11.79 |
| ATOM | 1095 | NE  | ARG | A | 141 | -2.697 | 41.124 | 62.834 | 1.00 | 18.11 |
| ATOM | 1096 | CZ  | ARG | A | 141 | -2.823 | 40.137 | 63.712 | 1.00 | 23.12 |
| ATOM | 1097 | NH1 | ARG | A | 141 | -3.704 | 40.177 | 64.695 | 1.00 | 16.74 |
| ATOM | 1098 | NH2 | ARG | A | 141 | -2.046 | 39.061 | 63.605 | 1.00 | 17.67 |
| ATOM | 1099 | N   | ALA | A | 142 | -2.326 | 45.981 | 59.695 | 1.00 | 22.16 |
| ATOM | 1100 | CA  | ALA | A | 142 | -2.572 | 47.406 | 59.886 | 1.00 | 21.34 |
| ATOM | 1101 | C   | ALA | A | 142 | -2.316 | 48.113 | 58.587 | 1.00 | 30.29 |
| ATOM | 1102 | O   | ALA | A | 142 | -2.436 | 49.334 | 58.521 | 1.00 | 28.98 |
| ATOM | 1103 | CB  | ALA | A | 142 | -1.797 | 48.097 | 61.022 | 1.00 | 18.86 |
| ATOM | 1104 | N   | ILE | A | 143 | -1.929 | 47.346 | 57.563 | 1.00 | 25.27 |
| ATOM | 1105 | CA  | ILE | A | 143 | -1.681 | 47.999 | 56.299 | 1.00 | 24.86 |
| ATOM | 1106 | C   | ILE | A | 143 | -2.654 | 47.464 | 55.249 | 1.00 | 33.21 |
| ATOM | 1107 | O   | ILE | A | 143 | -3.086 | 48.191 | 54.363 | 1.00 | 30.61 |
| ATOM | 1108 | CB  | ILE | A | 143 | -0.279 | 47.766 | 55.801 | 1.00 | 27.48 |
| ATOM | 1109 | CG1 | ILE | A | 143 | 0.735  | 48.464 | 56.683 | 1.00 | 25.48 |
| ATOM | 1110 | CG2 | ILE | A | 143 | -0.178 | 48.243 | 54.355 | 1.00 | 30.86 |
| ATOM | 1111 | CD1 | ILE | A | 143 | 2.134  | 48.057 | 56.257 | 1.00 | 21.10 |
| ATOM | 1112 | N   | LEU | A | 144 | -2.968 | 46.170 | 55.368 | 1.00 | 28.50 |
| ATOM | 1113 | CA  | LEU | A | 144 | -3.882 | 45.474 | 54.469 | 1.00 | 27.04 |
| ATOM | 1114 | C   | LEU | A | 144 | -4.383 | 44.197 | 55.122 | 1.00 | 31.13 |
| ATOM | 1115 | O   | LEU | A | 144 | -3.786 | 43.658 | 56.047 | 1.00 | 31.11 |
| ATOM | 1116 | CB  | LEU | A | 144 | -3.260 | 45.191 | 53.076 | 1.00 | 27.85 |
| ATOM | 1117 | CG  | LEU | A | 144 | -1.930 | 44.437 | 53.144 | 1.00 | 33.41 |
| ATOM | 1118 | CD1 | LEU | A | 144 | -2.147 | 42.925 | 53.111 | 1.00 | 34.28 |
| ATOM | 1119 | CD2 | LEU | A | 144 | -0.919 | 44.879 | 52.090 | 1.00 | 30.37 |
| ATOM | 1120 | N   | PRO | A | 145 | -5.499 | 43.703 | 54.628 | 1.00 | 28.27 |
| ATOM | 1121 | CA  | PRO | A | 145 | -6.113 | 42.489 | 55.143 | 1.00 | 25.97 |
| ATOM | 1122 | C   | PRO | A | 145 | -5.306 | 41.275 | 54.704 | 1.00 | 25.80 |
| ATOM | 1123 | O   | PRO | A | 145 | -4.911 | 41.145 | 53.543 | 1.00 | 26.89 |
| ATOM | 1124 | CB  | PRO | A | 145 | -7.527 | 42.445 | 54.533 | 1.00 | 25.97 |
| ATOM | 1125 | CG  | PRO | A | 145 | -7.710 | 43.760 | 53.795 | 1.00 | 30.32 |
| ATOM | 1126 | CD  | PRO | A | 145 | -6.334 | 44.377 | 53.597 | 1.00 | 26.43 |
| ATOM | 1127 | N   | CYS | A | 146 | -5.069 | 40.391 | 55.649 | 1.00 | 23.44 |
| ATOM | 1128 | CA  | CYS | A | 146 | -4.275 | 39.215 | 55.366 | 1.00 | 22.20 |
| ATOM | 1129 | C   | CYS | A | 146 | -4.338 | 38.173 | 56.478 | 1.00 | 25.91 |
| ATOM | 1130 | O   | CYS | A | 146 | -4.902 | 38.365 | 57.556 | 1.00 | 24.21 |
| ATOM | 1131 | CB  | CYS | A | 146 | -2.794 | 39.660 | 55.211 | 1.00 | 22.20 |
| ATOM | 1    |     |     |   |     |        |        |        |      |       |







|      |      |     |     |   |     |       |        |        |      |       |
|------|------|-----|-----|---|-----|-------|--------|--------|------|-------|
| ATOM | 1205 | CB  | TYR | A | 156 | 3.525 | 40.115 | 47.183 | 1.00 | 27.00 |
| ATOM | 1206 | CG  | TYR | A | 156 | 4.670 | 41.016 | 47.641 | 1.00 | 27.39 |
| ATOM | 1207 | CD1 | TYR | A | 156 | 4.801 | 42.315 | 47.146 | 1.00 | 30.16 |
| ATOM | 1208 | CD2 | TYR | A | 156 | 5.595 | 40.604 | 48.607 | 1.00 | 25.30 |
| ATOM | 1209 | CE1 | TYR | A | 156 | 5.821 | 43.164 | 47.579 | 1.00 | 33.17 |
| ATOM | 1210 | CE2 | TYR | A | 156 | 6.619 | 41.443 | 49.051 | 1.00 | 25.54 |
| ATOM | 1211 | CZ  | TYR | A | 156 | 6.732 | 42.746 | 48.553 | 1.00 | 39.24 |
| ATOM | 1212 | OH  | TYR | A | 156 | 7.722 | 43.618 | 49.005 | 1.00 | 26.94 |
| ATOM | 1213 | N   | THR | A | 157 | 3.468 | 41.057 | 44.314 | 1.00 | 25.18 |
| ATOM | 1214 | CA  | THR | A | 157 | 3.850 | 42.069 | 43.361 | 1.00 | 26.36 |
| ATOM | 1215 | C   | THR | A | 157 | 3.121 | 43.339 | 43.762 | 1.00 | 26.72 |
| ATOM | 1216 | O   | THR | A | 157 | 2.006 | 43.287 | 44.271 | 1.00 | 29.15 |
| ATOM | 1217 | CB  | THR | A | 157 | 3.556 | 41.663 | 41.903 | 1.00 | 38.57 |
| ATOM | 1218 | OG1 | THR | A | 157 | 2.297 | 41.030 | 41.834 | 1.00 | 38.99 |
| ATOM | 1219 | CG2 | THR | A | 157 | 4.639 | 40.682 | 41.499 | 1.00 | 35.90 |
| ATOM | 1220 | N   | ALA | A | 158 | 3.753 | 44.470 | 43.552 | 1.00 | 28.59 |
| ATOM | 1221 | CA  | ALA | A | 158 | 3.100 | 45.700 | 43.942 | 1.00 | 33.23 |
| ATOM | 1222 | C   | ALA | A | 158 | 3.495 | 46.868 | 43.051 | 1.00 | 37.76 |
| ATOM | 1223 | O   | ALA | A | 158 | 4.598 | 46.946 | 42.482 | 1.00 | 35.09 |
| ATOM | 1224 | CB  | ALA | A | 158 | 3.487 | 46.038 | 45.382 | 1.00 | 34.39 |
| ATOM | 1225 | N   | GLU | A | 159 | 2.557 | 47.793 | 42.962 | 1.00 | 36.52 |
| ATOM | 1226 | CA  | GLU | A | 159 | 2.779 | 49.011 | 42.213 | 1.00 | 38.54 |
| ATOM | 1227 | C   | GLU | A | 159 | 2.305 | 50.109 | 43.125 | 1.00 | 33.69 |
| ATOM | 1228 | O   | GLU | A | 159 | 1.204 | 50.050 | 43.690 | 1.00 | 29.21 |
| ATOM | 1229 | CB  | GLU | A | 159 | 2.119 | 49.064 | 40.829 | 1.00 | 42.31 |
| ATOM | 1230 | CG  | GLU | A | 159 | 1.120 | 47.914 | 40.600 | 1.00 | 75.57 |
| ATOM | 1231 | CD  | GLU | A | 159 | 1.146 | 47.437 | 39.182 | 1.00 | 99.03 |
| ATOM | 1232 | OE1 | GLU | A | 159 | 0.467 | 47.937 | 38.296 | 1.00 | 77.74 |
| ATOM | 1233 | OE2 | GLU | A | 159 | 2.010 | 46.464 | 39.021 | 1.00 | 90.11 |
| ATOM | 1234 | N   | VAL | A | 160 | 3.181 | 51.064 | 43.345 | 1.00 | 30.74 |
| ATOM | 1235 | CA  | VAL | A | 160 | 2.726 | 52.053 | 44.289 | 1.00 | 32.22 |
| ATOM | 1236 | C   | VAL | A | 160 | 2.872 | 53.454 | 43.745 | 1.00 | 36.18 |
| ATOM | 1237 | O   | VAL | A | 160 | 3.942 | 53.801 | 43.239 | 1.00 | 32.54 |
| ATOM | 1238 | CB  | VAL | A | 160 | 3.367 | 51.832 | 45.665 | 1.00 | 31.25 |
| ATOM | 1239 | CG1 | VAL | A | 160 | 4.614 | 50.978 | 45.535 | 1.00 | 32.36 |
| ATOM | 1240 | CG2 | VAL | A | 160 | 3.697 | 53.130 | 46.385 | 1.00 | 27.21 |
| ATOM | 1241 | N   | SER | A | 161 | 1.776 | 54.222 | 43.839 | 1.00 | 34.59 |
| ATOM | 1242 | CA  | SER | A | 161 | 1.825 | 55.583 | 43.353 | 1.00 | 33.57 |
| ATOM | 1243 | C   | SER | A | 161 | 2.245 | 56.562 | 44.417 | 1.00 | 35.27 |
| ATOM | 1244 | O   | SER | A | 161 | 1.623 | 56.619 | 45.487 | 1.00 | 31.96 |
| ATOM | 1245 | CB  | SER | A | 161 | 0.547 | 56.111 | 42.745 | 1.00 | 33.76 |
| ATOM | 1246 | OG  | SER | A | 161 | 0.919 | 57.320 | 42.106 | 1.00 | 38.24 |
| ATOM | 1247 | N   | VAL | A | 162 | 3.285 | 57.313 | 44.054 | 1.00 | 35.28 |



|      |      |     |     |   |     |        |        |        |      |        |
|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
| ATOM | 1263 | C   | LYS | A | 164 | 8.111  | 62.681 | 42.151 | 1.00 | 46.24  |
| ATOM | 1264 | O   | LYS | A | 164 | 9.119  | 62.088 | 41.784 | 1.00 | 46.96  |
| ATOM | 1265 | CB  | LYS | A | 164 | 6.556  | 63.551 | 40.440 | 1.00 | 55.91  |
| ATOM | 1266 | CG  | LYS | A | 164 | 5.133  | 63.813 | 39.942 | 1.00 | 97.37  |
| ATOM | 1267 | CD  | LYS | A | 164 | 5.012  | 64.953 | 38.913 | 1.00 | 100.00 |
| ATOM | 1268 | CE  | LYS | A | 164 | 5.120  | 64.558 | 37.434 | 1.00 | 100.00 |
| ATOM | 1269 | NZ  | LYS | A | 164 | 3.833  | 64.450 | 36.718 | 1.00 | 100.00 |
| ATOM | 1270 | N   | GLU | A | 165 | 8.164  | 63.595 | 43.102 | 1.00 | 42.61  |
| ATOM | 1271 | CA  | GLU | A | 165 | 9.422  | 63.941 | 43.749 | 1.00 | 45.37  |
| ATOM | 1272 | C   | GLU | A | 165 | 10.005 | 62.929 | 44.747 | 1.00 | 47.34  |
| ATOM | 1273 | O   | GLU | A | 165 | 11.156 | 63.001 | 45.179 | 1.00 | 43.70  |
| ATOM | 1274 | CB  | GLU | A | 165 | 9.349  | 65.366 | 44.343 | 1.00 | 47.53  |
| ATOM | 1275 | CG  | GLU | A | 165 | 8.275  | 65.541 | 45.446 | 1.00 | 66.49  |
| ATOM | 1276 | CD  | GLU | A | 165 | 6.837  | 65.640 | 44.991 | 1.00 | 96.79  |
| ATOM | 1277 | OE1 | GLU | A | 165 | 6.436  | 65.365 | 43.864 | 1.00 | 99.56  |
| ATOM | 1278 | OE2 | GLU | A | 165 | 6.056  | 66.058 | 45.964 | 1.00 | 77.24  |
| ATOM | 1279 | N   | LEU | A | 166 | 9.197  | 61.958 | 45.118 | 1.00 | 44.94  |
| ATOM | 1280 | CA  | LEU | A | 166 | 9.647  | 60.996 | 46.084 | 1.00 | 40.65  |
| ATOM | 1281 | C   | LEU | A | 166 | 9.908  | 59.636 | 45.497 | 1.00 | 50.07  |
| ATOM | 1282 | O   | LEU | A | 166 | 9.354  | 59.307 | 44.443 | 1.00 | 52.03  |
| ATOM | 1283 | CB  | LEU | A | 166 | 8.566  | 60.917 | 47.170 | 1.00 | 35.62  |
| ATOM | 1284 | CG  | LEU | A | 166 | 8.264  | 62.286 | 47.766 | 1.00 | 31.47  |
| ATOM | 1285 | CD1 | LEU | A | 166 | 7.234  | 62.081 | 48.848 | 1.00 | 29.41  |
| ATOM | 1286 | CD2 | LEU | A | 166 | 9.521  | 62.927 | 48.364 | 1.00 | 25.32  |
| ATOM | 1287 | N   | VAL | A | 167 | 10.744 | 58.884 | 46.229 | 1.00 | 43.25  |
| ATOM | 1288 | CA  | VAL | A | 167 | 11.112 | 57.508 | 45.933 | 1.00 | 39.13  |
| ATOM | 1289 | C   | VAL | A | 167 | 10.432 | 56.490 | 46.855 | 1.00 | 44.52  |
| ATOM | 1290 | O   | VAL | A | 167 | 10.327 | 56.679 | 48.074 | 1.00 | 39.15  |
| ATOM | 1291 | CB  | VAL | A | 167 | 12.592 | 57.293 | 46.083 | 1.00 | 37.94  |
| ATOM | 1292 | CG1 | VAL | A | 167 | 12.920 | 55.922 | 45.515 | 1.00 | 35.52  |
| ATOM | 1293 | CG2 | VAL | A | 167 | 13.303 | 58.401 | 45.345 | 1.00 | 37.13  |
| ATOM | 1294 | N   | ALA | A | 168 | 9.998  | 55.394 | 46.233 | 1.00 | 39.32  |
| ATOM | 1295 | CA  | ALA | A | 168 | 9.363  | 54.288 | 46.918 | 1.00 | 34.98  |
| ATOM | 1296 | C   | ALA | A | 168 | 10.209 | 53.034 | 46.762 | 1.00 | 40.61  |
| ATOM | 1297 | O   | ALA | A | 168 | 10.720 | 52.782 | 45.671 | 1.00 | 40.08  |
| ATOM | 1298 | CB  | ALA | A | 168 | 7.957  | 54.003 | 46.427 | 1.00 | 33.16  |
| ATOM | 1299 | N   | LEU | A | 169 | 10.380 | 52.295 | 47.876 | 1.00 | 32.03  |
| ATOM | 1300 | CA  | LEU | A | 169 | 11.104 | 51.038 | 47.926 | 1.00 | 27.11  |
| ATOM | 1301 | C   | LEU | A | 169 | 10.289 | 50.039 | 48.717 | 1.00 | 32.61  |
| ATOM | 1302 | O   | LEU | A | 169 | 9.460  | 50.400 | 49.544 | 1.00 | 33.15  |
| ATOM | 1303 | CB  | LEU | A | 169 | 12.543 | 51.071 | 48.449 | 1.00 | 25.35  |
| ATOM | 1304 | CG  | LEU | A | 169 | 13.362 | 52.250 | 47.964 | 1.00 | 29.91  |
| ATOM | 1305 | CD1 | LEU | A | 169 | 14.686 | 52.206 | 48.708 | 1.00 | 29.99  |
| ATOM | 1306 | CD2 | LEU | A | 169 | 13.676 | 52.118 | 46.482 | 1.00 | 29.66  |
| ATOM | 1307 | N   | MET | A | 170 | 10.495 | 48.764 | 48.417 | 1.00 | 31.01  |
| ATOM | 1308 | CA  | MET | A | 170 | 9.811  | 47.680 | 49.081 | 1.00 | 25.79  |
| ATOM | 1309 | C   | MET | A | 170 | 10.757 | 46.537 | 49.309 | 1.00 | 24.72  |
| ATOM | 1310 | O   | MET | A | 170 | 11.896 | 46.474 | 48.835 | 1.00 | 23.26  |
| ATOM | 1311 | CB  | MET | A | 170 | 8.569  | 47.164 | 48.337 | 1.00 | 28.25  |
| ATOM | 1312 | CG  | MET | A | 170 | 7.556  | 48.274 | 48.171 | 1.00 | 31.25  |
| ATOM | 1313 | SD  | MET | A | 170 | 5.901  | 47.652 | 47.812 | 1.00 | 35.46  |
| ATOM | 1314 | CE  | MET | A | 170 | 5.341  | 46.854 | 49.347 | 1.00 | 30.63  |
| ATOM | 1315 | N   | SER | A | 171 | 10.265 | 45.599 | 50.078 | 1.00 | 25.49  |
| ATOM | 1316 | CA  | SER | A | 171 | 11.080 | 44.433 | 50.331 | 1.00 | 23.48  |
| ATOM | 1317 | C   | SER | A | 171 | 10.947 | 43.519 | 49.087 | 1.00 | 26.82  |
| ATOM | 1318 | O   | SER | A | 171 | 10.414 | 42.426 | 49.110 | 1.00 | 22.63  |
| ATOM | 1319 | CB  | SER | A | 171 | 10.623 | 43.790 | 51.641 | 1.00 | 18.95  |
| ATOM | 1320 | OG  | SER | A | 171 | 9.230  | 43.521 | 51.646 | 1.00 | 24.18  |



|      |      |     |     |   |     |        |        |          |      |       |
|------|------|-----|-----|---|-----|--------|--------|----------|------|-------|
| ATOM | 1321 | N   | ALA | A | 172 | 11.378 | 43.996 | 47.944   | 1.00 | 28.35 |
| ATOM | 1322 | CA  | ALA | A | 172 | 11.234 | 43.201 | 46.752   | 1.00 | 28.47 |
| ATOM | 1323 | C   | ALA | A | 172 | 12.201 | 43.688 | 45.722   | 1.00 | 31.99 |
| ATOM | 1324 | O   | ALA | A | 172 | 12.997 | 44.593 | 45.971   | 1.00 | 30.63 |
| ATOM | 1325 | CB  | ALA | A | 172 | 9.829  | 43.376 | 46.201   | 1.00 | 29.09 |
| ATOM | 1326 | N   | ILE | A | 173 | 12.116 | 43.086 | 44.546   | 1.00 | 34.66 |
| ATOM | 1327 | CA  | ILE | A | 173 | 12.998 | 43.523 | 43.461   | 1.00 | 34.83 |
| ATOM | 1328 | C   | ILE | A | 173 | 12.335 | 44.698 | 42.748   | 1.00 | 30.47 |
| ATOM | 1329 | O   | ILE | A | 173 | 11.131 | 44.679 | 42.428   | 1.00 | 26.31 |
| ATOM | 1330 | CB  | ILE | A | 173 | 13.395 | 42.387 | 42.489   | 1.00 | 39.22 |
| ATOM | 1331 | CG1 | ILE | A | 173 | 14.129 | 41.209 | 43.136   | 1.00 | 36.75 |
| ATOM | 1332 | CG2 | ILE | A | 173 | 14.187 | 42.873 | 41.289   | 1.00 | 44.70 |
| ATOM | 1333 | CD1 | ILE | A | 173 | 15.550 | 41.465 | 43.629   | 1.00 | 30.83 |
| ATOM | 1334 | N   | ARG | A | 174 | 13.099 | 45.770 | 42.566   | 1.00 | 34.59 |
| ATOM | 1335 | CA  | ARG | A | 174 | 12.570 | 46.949 | 41.885   | 1.00 | 38.22 |
| ATOM | 1336 | C   | ARG | A | 174 | 12.357 | 46.486 | 40.452   | 1.00 | 53.38 |
| ATOM | 1337 | O   | ARG | A | 174 | 13.316 | 46.011 | 39.836   | 1.00 | 51.64 |
| ATOM | 1338 | CB  | ARG | A | 174 | 13.605 | 48.057 | 41.889   | 1.00 | 33.91 |
| ATOM | 1339 | CG  | ARG | A | 174 | 13.671 | 48.862 | 43.182   | 1.00 | 39.95 |
| ATOM | 1340 | CD  | ARG | A | 174 | 14.912 | 49.754 | 43.233   | 1.00 | 34.61 |
| ATOM | 1341 | NE  | ARG | A | 174 | 16.083 | 49.015 | 43.674   | 1.00 | 62.75 |
| ATOM | 1342 | CZ  | ARG | A | 174 | 17.292 | 49.144 | 43.151   | 1.00 | 81.12 |
| ATOM | 1343 | NH1 | ARG | A | 174 | 17.505 | 50.000 | 42.133   | 1.00 | 38.29 |
| ATOM | 1344 | NH2 | ARG | A | 174 | 18.276 | 48.393 | 43.686   | 1.00 | 52.86 |
| ATOM | 1345 | N   | ASP | A | 175 | 11.119 | 46.550 | 39.968   | 1.00 | 59.05 |
| ATOM | 1346 | CA  | ASP | A | 175 | 10.801 | 46.044 | 38.640   | 1.00 | 65.93 |
| ATOM | 1347 | C   | ASP | A | 175 | 10.737 | 47.100 | 37.551   | 1.00 | 83.82 |
| ATOM | 1348 | O   | ASP | A | 175 | 10.852 | 46.833 | 36.342   | 1.00 | 91.77 |
| ATOM | 1349 | CB  | ASP | A | 175 | 9.567  | 45.123 | 38.677   | 1.00 | 67.87 |
| ATOM | 1350 | CG  | ASP | A | 175 | 9.102  | 44.615 | 37.340   | 1.00 | 73.42 |
| ATOM | 1351 | OD1 | ASP | A | 175 | 9.855  | 44.262 | 36.438   | 1.00 | 75.53 |
| ATOM | 1352 | OD2 | ASP | A | 175 | 7.785  | 44.579 | 37.288   | 1.00 | 72.28 |
| ATOM | 1353 | N   | GLY | A | 176 | 10.553 | 48.327 | 38.002   | 1.00 | 77.53 |
| ATOM | 1354 | CA  | GLY | A | 176 | 10.469 | 49.438 | 37.089   | 1.00 | 77.66 |
| ATOM | 1355 | C   | GLY | A | 176 | 9.804  | 50.660 | 37.704   | 1.00 | 82.05 |
| ATOM | 1356 | O   | GLY | A | 176 | 9.128  | 50.560 | 38.731   | 1.00 | 79.00 |
| ATOM | 1357 | N   | GLU | A | 177 | 9.995  | 51.815 | 37.044   | 1.00 | 81.79 |
| ATOM | 1358 | CA  | GLU | A | 177 | 9.441  | 53.110 | 37.460   | 1.00 | 81.14 |
| ATOM | 1359 | C   | GLU | A | 177 | 8.800  | 53.917 | 36.333   | 1.00 | 86.27 |
| ATOM | 1360 | O   | GLU | A | 177 | 9.419  | 54.218 | 35.313   | 1.00 | 88.04 |
| ATOM | 1361 | CB  | GLU | A | 177 | 10.468 | 53.977 | 38.210   | 1.00 | 82.57 |
| ATOM | 1362 | CG  | GLU | A | 177 | 11.115 | 55.073 | 37.340   | 1.00 | 93.83 |
| ATOM | 1363 | CD  | GLU | A | 177 | 11.662 | 56.220 | 38.142</ |      |       |



|      |      |     |     |   |     |        |        |        |      |        |
|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
| ATOM | 1379 | CD  | PRO | A | 179 | 6.791  | 57.663 | 34.270 | 1.00 | 80.56  |
| ATOM | 1380 | N   | ASP | A | 180 | 2.597  | 58.025 | 36.405 | 1.00 | 66.91  |
| ATOM | 1381 | CA  | ASP | A | 180 | 1.242  | 57.625 | 36.543 | 1.00 | 66.81  |
| ATOM | 1382 | C   | ASP | A | 180 | 0.510  | 58.373 | 35.459 | 1.00 | 86.40  |
| ATOM | 1383 | O   | ASP | A | 180 | 1.063  | 59.307 | 34.883 | 1.00 | 89.77  |
| ATOM | 1384 | CB  | ASP | A | 180 | 0.808  | 58.093 | 37.946 | 1.00 | 63.63  |
| ATOM | 1385 | CG  | ASP | A | 180 | -0.408 | 57.401 | 38.482 | 1.00 | 74.66  |
| ATOM | 1386 | OD1 | ASP | A | 180 | -0.968 | 56.519 | 37.870 | 1.00 | 83.41  |
| ATOM | 1387 | OD2 | ASP | A | 180 | -0.812 | 57.829 | 39.655 | 1.00 | 69.97  |
| ATOM | 1388 | N   | PRO | A | 181 | -0.732 | 57.992 | 35.187 | 1.00 | 90.42  |
| ATOM | 1389 | CA  | PRO | A | 181 | -1.584 | 58.645 | 34.218 | 1.00 | 91.10  |
| ATOM | 1390 | C   | PRO | A | 181 | -2.945 | 58.619 | 34.873 | 1.00 | 91.79  |
| ATOM | 1391 | O   | PRO | A | 181 | -3.748 | 57.724 | 34.638 | 1.00 | 87.89  |
| ATOM | 1392 | CB  | PRO | A | 181 | -1.541 | 57.787 | 32.929 | 1.00 | 94.08  |
| ATOM | 1393 | CG  | PRO | A | 181 | -0.582 | 56.635 | 33.200 | 1.00 | 98.94  |
| ATOM | 1394 | CD  | PRO | A | 181 | -0.115 | 56.760 | 34.655 | 1.00 | 92.93  |
| ATOM | 1395 | N   | GLU | A | 182 | -3.175 | 59.556 | 35.793 | 1.00 | 88.82  |
| ATOM | 1396 | CA  | GLU | A | 182 | -4.443 | 59.519 | 36.506 | 1.00 | 89.31  |
| ATOM | 1397 | C   | GLU | A | 182 | -4.808 | 60.809 | 37.218 | 1.00 | 98.64  |
| ATOM | 1398 | O   | GLU | A | 182 | -5.181 | 60.787 | 38.385 | 1.00 | 99.08  |
| ATOM | 1399 | CB  | GLU | A | 182 | -4.359 | 58.380 | 37.528 | 1.00 | 90.42  |
| ATOM | 1400 | CG  | GLU | A | 182 | -5.510 | 57.373 | 37.391 | 1.00 | 98.92  |
| ATOM | 1401 | CD  | GLU | A | 182 | -6.826 | 58.010 | 37.750 | 1.00 | 100.00 |
| ATOM | 1402 | OE1 | GLU | A | 182 | -7.465 | 58.719 | 36.986 | 1.00 | 100.00 |
| ATOM | 1403 | OE2 | GLU | A | 182 | -7.169 | 57.806 | 39.003 | 1.00 | 100.00 |
| ATOM | 1404 | N   | ASP | A | 183 | -4.704 | 61.939 | 36.487 | 1.00 | 100.00 |
| ATOM | 1405 | CA  | ASP | A | 183 | -4.952 | 63.289 | 37.021 | 1.00 | 100.00 |
| ATOM | 1406 | C   | ASP | A | 183 | -4.112 | 63.534 | 38.264 | 1.00 | 100.00 |
| ATOM | 1407 | O   | ASP | A | 183 | -4.557 | 64.229 | 39.192 | 1.00 | 100.00 |
| ATOM | 1408 | CB  | ASP | A | 183 | -6.460 | 63.709 | 37.195 | 1.00 | 100.00 |
| ATOM | 1409 | CG  | ASP | A | 183 | -7.509 | 62.613 | 37.228 | 1.00 | 100.00 |
| ATOM | 1410 | OD1 | ASP | A | 183 | -8.091 | 62.209 | 36.225 | 1.00 | 100.00 |
| ATOM | 1411 | OD2 | ASP | A | 183 | -7.745 | 62.155 | 38.451 | 1.00 | 100.00 |
| ATOM | 1412 | N   | PRO | A | 184 | -2.878 | 62.960 | 38.272 | 1.00 | 97.37  |
| ATOM | 1413 | CA  | PRO | A | 184 | -2.075 | 63.104 | 39.462 | 1.00 | 95.12  |
| ATOM | 1414 | C   | PRO | A | 184 | -0.708 | 63.687 | 39.190 | 1.00 | 98.12  |
| ATOM | 1415 | O   | PRO | A | 184 | -0.248 | 63.872 | 38.049 | 1.00 | 96.48  |
| ATOM | 1416 | CB  | PRO | A | 184 | -1.735 | 61.635 | 39.703 | 1.00 | 96.33  |
| ATOM | 1417 | CG  | PRO | A | 184 | -1.335 | 61.138 | 38.314 | 1.00 | 100.00 |
| ATOM | 1418 | CD  | PRO | A | 184 | -2.110 | 62.028 | 37.363 | 1.00 | 96.08  |
| ATOM | 1419 | N   | SER | A | 185 | -0.023 | 63.913 | 40.311 | 1.00 | 92.79  |
| ATOM | 1420 | CA  | SER | A | 185 | 1.347  | 64.393 | 40.313 | 1.00 | 88.74  |
| ATOM | 1421 | C   | SER | A | 185 | 2.206  | 63.348 | 41.012 | 1.00 | 81.94  |
| ATOM | 1422 | O   | SER | A | 185 | 3.066  | 63.667 | 41.846 | 1.00 | 84.44  |
| ATOM | 1423 | CB  | SER | A | 185 | 1.541  | 65.771 | 40.914 | 1.00 | 93.34  |
| ATOM | 1424 | OG  | SER | A | 185 | 2.614  | 66.419 | 40.251 | 1.00 | 100.00 |
| ATOM | 1425 | N   | ARG | A | 186 | 1.930  | 62.095 | 40.627 | 1.00 | 64.19  |
| ATOM | 1426 | CA  | ARG | A | 186 | 2.596  | 60.947 | 41.162 | 1.00 | 59.49  |
| ATOM | 1427 | C   | ARG | A | 186 | 3.282  | 60.116 | 40.116 | 1.00 | 59.45  |
| ATOM | 1428 | O   | ARG | A | 186 | 3.053  | 60.227 | 38.916 | 1.00 | 59.05  |
| ATOM | 1429 | CB  | ARG | A | 186 | 1.659  | 60.042 | 41.958 | 1.00 | 55.86  |
| ATOM | 1430 | CG  | ARG | A | 186 | 0.324  | 60.675 | 42.291 | 1.00 | 27.25  |
| ATOM | 1431 | CD  | ARG | A | 186 | -0.548 | 59.827 | 43.204 | 1.00 | 57.78  |
| ATOM | 1432 | NE  | ARG | A | 186 | 0.194  | 59.220 | 44.306 | 1.00 | 80.89  |
| ATOM | 1433 | CZ  | ARG | A | 186 | 0.569  | 59.842 | 45.420 | 1.00 | 97.56  |
| ATOM | 1434 | NH1 | ARG | A | 186 | 0.297  | 61.124 | 45.643 | 1.00 | 83.79  |
| ATOM | 1435 | NH2 | ARG | A | 186 | 1.235  | 59.142 | 46.335 | 1.00 | 85.34  |
| ATOM | 1436 | N   | LYS | A | 187 | 4.128  | 59.268 | 40.675 | 1.00 | 53.71  |



|      |      |     |     |   |     |        |        |        |      |        |
|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
| ATOM | 1437 | CA  | LYS | A | 187 | 4.904  | 58.295 | 39.970 | 1.00 | 50.62  |
| ATOM | 1438 | C   | LYS | A | 187 | 4.359  | 56.988 | 40.450 | 1.00 | 53.26  |
| ATOM | 1439 | O   | LYS | A | 187 | 3.776  | 56.881 | 41.543 | 1.00 | 51.61  |
| ATOM | 1440 | CB  | LYS | A | 187 | 6.351  | 58.266 | 40.393 | 1.00 | 52.26  |
| ATOM | 1441 | CG  | LYS | A | 187 | 7.282  | 59.118 | 39.571 | 1.00 | 54.27  |
| ATOM | 1442 | CD  | LYS | A | 187 | 8.703  | 58.584 | 39.606 | 1.00 | 55.39  |
| ATOM | 1443 | CE  | LYS | A | 187 | 9.728  | 59.611 | 40.051 | 1.00 | 31.63  |
| ATOM | 1444 | NZ  | LYS | A | 187 | 11.058 | 59.374 | 39.481 | 1.00 | 46.19  |
| ATOM | 1445 | N   | ILE | A | 188 | 4.598  | 56.025 | 39.584 | 1.00 | 49.44  |
| ATOM | 1446 | CA  | ILE | A | 188 | 4.200  | 54.683 | 39.845 | 1.00 | 48.00  |
| ATOM | 1447 | C   | ILE | A | 188 | 5.361  | 53.694 | 39.935 | 1.00 | 53.77  |
| ATOM | 1448 | O   | ILE | A | 188 | 6.057  | 53.436 | 38.951 | 1.00 | 53.51  |
| ATOM | 1449 | CB  | ILE | A | 188 | 2.753  | 54.307 | 39.572 | 1.00 | 49.99  |
| ATOM | 1450 | CG1 | ILE | A | 188 | 2.558  | 52.804 | 39.554 | 1.00 | 51.55  |
| ATOM | 1451 | CG2 | ILE | A | 188 | 2.229  | 54.973 | 38.315 | 1.00 | 51.74  |
| ATOM | 1452 | CD1 | ILE | A | 188 | 1.336  | 52.415 | 40.385 | 1.00 | 80.62  |
| ATOM | 1453 | N   | TYR | A | 189 | 5.640  | 53.226 | 41.166 | 1.00 | 45.90  |
| ATOM | 1454 | CA  | TYR | A | 189 | 6.742  | 52.322 | 41.402 | 1.00 | 40.92  |
| ATOM | 1455 | C   | TYR | A | 189 | 6.330  | 50.851 | 41.496 | 1.00 | 40.81  |
| ATOM | 1456 | O   | TYR | A | 189 | 5.362  | 50.493 | 42.188 | 1.00 | 39.23  |
| ATOM | 1457 | CB  | TYR | A | 189 | 7.528  | 52.773 | 42.638 | 1.00 | 40.24  |
| ATOM | 1458 | CG  | TYR | A | 189 | 8.427  | 53.968 | 42.455 | 1.00 | 31.23  |
| ATOM | 1459 | CD1 | TYR | A | 189 | 9.711  | 53.803 | 41.939 | 1.00 | 31.58  |
| ATOM | 1460 | CD2 | TYR | A | 189 | 8.046  | 55.239 | 42.886 | 1.00 | 30.59  |
| ATOM | 1461 | CE1 | TYR | A | 189 | 10.593 | 54.879 | 41.813 | 1.00 | 34.77  |
| ATOM | 1462 | CE2 | TYR | A | 189 | 8.913  | 56.328 | 42.764 | 1.00 | 31.23  |
| ATOM | 1463 | CZ  | TYR | A | 189 | 10.188 | 56.151 | 42.224 | 1.00 | 39.57  |
| ATOM | 1464 | OH  | TYR | A | 189 | 11.058 | 57.218 | 42.096 | 1.00 | 34.19  |
| ATOM | 1465 | N   | LYS | A | 190 | 7.123  | 50.034 | 40.775 | 1.00 | 39.37  |
| ATOM | 1466 | CA  | LYS | A | 190 | 6.971  | 48.589 | 40.627 | 1.00 | 39.51  |
| ATOM | 1467 | C   | LYS | A | 190 | 8.024  | 47.700 | 41.305 | 1.00 | 35.21  |
| ATOM | 1468 | O   | LYS | A | 190 | 9.235  | 47.928 | 41.275 | 1.00 | 32.65  |
| ATOM | 1469 | CB  | LYS | A | 190 | 6.775  | 48.214 | 39.161 | 1.00 | 43.13  |
| ATOM | 1470 | CG  | LYS | A | 190 | 5.359  | 48.468 | 38.642 | 1.00 | 68.06  |
| ATOM | 1471 | CD  | LYS | A | 190 | 5.308  | 49.170 | 37.290 | 1.00 | 80.52  |
| ATOM | 1472 | CE  | LYS | A | 190 | 5.559  | 48.262 | 36.089 | 1.00 | 100.00 |
| ATOM | 1473 | NZ  | LYS | A | 190 | 6.556  | 48.792 | 35.135 | 1.00 | 100.00 |
| ATOM | 1474 | N   | PHE | A | 191 | 7.502  | 46.641 | 41.907 | 1.00 | 32.67  |
| ATOM | 1475 | CA  | PHE | A | 191 | 8.296  | 45.679 | 42.651 | 1.00 | 31.95  |
| ATOM | 1476 | C   | PHE | A | 191 | 7.784  | 44.249 | 42.523 | 1.00 | 33.46  |
| ATOM | 1477 | O   | PHE | A | 191 | 6.571  | 43.970 | 42.462 | 1.00 | 32.26  |
| ATOM | 1478 | CB  | PHE | A | 191 | 8.182  | 46.052 | 44.157 | 1.00 | 31.15  |
| ATOM | 1479 | CG  | PHE | A | 191 | 8.495  | 47.505 | 44.457 | 1.00 | 25.52  |
| ATOM | 1480 | CD1 | PHE | A | 191 | 9.813  | 47.930 | 44.618 | 1.00 | 25.46  |
| ATOM | 1481 | CD2 | PHE | A | 191 | 7.477  | 48.447 | 44.582 | 1.00 | 28.24  |
| ATOM | 1482 | CE1 | PHE | A | 191 | 10.131 | 49.261 | 44.884 | 1.00 | 27.83  |
| ATOM | 1483 | CE2 | PHE | A | 191 | 7.769  | 49.786 | 44.841 | 1.00 | 30.83  |
| ATOM | 1484 | CZ  | PHE | A | 191 | 9.095  | 50.188 | 44.999 | 1.00 | 29.60  |
| ATOM | 1485 | N   | ILE | A | 192 | 8.732  | 43.324 | 42.567 | 1.00 | 33.50  |
| ATOM | 1486 | CA  | ILE | A | 192 | 8.358  | 41.918 | 42.502 | 1.00 | 35.54  |
| ATOM | 1487 | C   | ILE | A | 192 | 9.089  | 41.083 | 43.523 | 1.00 | 27.79  |
| ATOM | 1488 | O   | ILE | A | 192 | 10.299 | 41.147 | 43.644 | 1.00 | 26.68  |
| ATOM | 1489 | CB  | ILE | A | 192 | 8.521  | 41.221 | 41.133 | 1.00 | 40.49  |
| ATOM | 1490 | CG1 | ILE | A | 192 | 9.982  | 41.182 | 40.709 | 1.00 | 43.06  |
| ATOM | 1491 | CG2 | ILE | A | 192 | 7.753  | 41.957 | 40.052 | 1.00 | 44.56  |
| ATOM | 1492 | CD1 | ILE | A | 192 | 10.729 | 39.903 | 41.096 | 1.00 | 83.58  |
| ATOM | 1493 | N   | GLN | A | 193 | 8.322  | 40.266 | 44.204 | 1.00 | 29.76  |
| ATOM | 1494 | CA  | GLN | A | 193 | 8.903  | 39.386 | 45.177 | 1.00 | 30.86  |



|      |      |     |           |        |        |        |      |       |
|------|------|-----|-----------|--------|--------|--------|------|-------|
| ATOM | 1495 | C   | GLN A 193 | 8.505  | 37.983 | 44.831 | 1.00 | 28.66 |
| ATOM | 1496 | O   | GLN A 193 | 7.406  | 37.529 | 45.181 | 1.00 | 27.73 |
| ATOM | 1497 | CB  | GLN A 193 | 8.625  | 39.729 | 46.669 | 1.00 | 32.91 |
| ATOM | 1498 | CG  | GLN A 193 | 9.339  | 38.787 | 47.682 | 1.00 | 24.21 |
| ATOM | 1499 | CD  | GLN A 193 | 10.864 | 38.777 | 47.631 | 1.00 | 20.52 |
| ATOM | 1500 | OE1 | GLN A 193 | 11.448 | 37.867 | 47.031 | 1.00 | 28.37 |
| ATOM | 1501 | NE2 | GLN A 193 | 11.535 | 39.752 | 48.272 | 1.00 | 21.68 |
| ATOM | 1502 | N   | LYS A 194 | 9.477  | 37.342 | 44.163 | 1.00 | 30.49 |
| ATOM | 1503 | CA  | LYS A 194 | 9.401  | 35.950 | 43.684 | 1.00 | 34.51 |
| ATOM | 1504 | C   | LYS A 194 | 9.563  | 34.882 | 44.787 | 1.00 | 40.98 |
| ATOM | 1505 | O   | LYS A 194 | 9.071  | 33.753 | 44.652 | 1.00 | 39.86 |
| ATOM | 1506 | CB  | LYS A 194 | 10.319 | 35.663 | 42.485 | 1.00 | 36.96 |
| ATOM | 1507 | CG  | LYS A 194 | 9.652  | 35.946 | 41.148 | 1.00 | 60.69 |
| ATOM | 1508 | CD  | LYS A 194 | 10.655 | 36.201 | 40.037 | 1.00 | 71.49 |
| ATOM | 1509 | CE  | LYS A 194 | 10.024 | 36.595 | 38.711 | 1.00 | 70.55 |
| ATOM | 1510 | NZ  | LYS A 194 | 11.032 | 37.075 | 37.745 | 1.00 | 96.02 |
| ATOM | 1511 | N   | VAL A 195 | 10.268 | 35.201 | 45.882 | 1.00 | 28.85 |
| ATOM | 1512 | CA  | VAL A 195 | 10.383 | 34.203 | 46.929 | 1.00 | 24.96 |
| ATOM | 1513 | C   | VAL A 195 | 9.195  | 34.303 | 47.895 | 1.00 | 28.79 |
| ATOM | 1514 | O   | VAL A 195 | 8.820  | 35.398 | 48.331 | 1.00 | 30.73 |
| ATOM | 1515 | CB  | VAL A 195 | 11.716 | 34.313 | 47.649 | 1.00 | 28.17 |
| ATOM | 1516 | CG1 | VAL A 195 | 11.907 | 33.002 | 48.380 | 1.00 | 31.42 |
| ATOM | 1517 | CG2 | VAL A 195 | 12.875 | 34.513 | 46.672 | 1.00 | 26.41 |
| ATOM | 1518 | N   | PRO A 196 | 8.540  | 33.179 | 48.222 | 1.00 | 23.07 |
| ATOM | 1519 | CA  | PRO A 196 | 7.423  | 33.248 | 49.134 | 1.00 | 20.29 |
| ATOM | 1520 | C   | PRO A 196 | 7.931  | 33.653 | 50.519 | 1.00 | 26.98 |
| ATOM | 1521 | O   | PRO A 196 | 8.932  | 33.121 | 51.013 | 1.00 | 23.36 |
| ATOM | 1522 | CB  | PRO A 196 | 6.769  | 31.869 | 49.189 | 1.00 | 19.98 |
| ATOM | 1523 | CG  | PRO A 196 | 7.665  | 30.923 | 48.414 | 1.00 | 24.10 |
| ATOM | 1524 | CD  | PRO A 196 | 8.673  | 31.798 | 47.691 | 1.00 | 23.37 |
| ATOM | 1525 | N   | ILE A 197 | 7.254  | 34.639 | 51.105 | 1.00 | 25.17 |
| ATOM | 1526 | CA  | ILE A 197 | 7.642  | 35.141 | 52.407 | 1.00 | 22.96 |
| ATOM | 1527 | C   | ILE A 197 | 6.431  | 35.273 | 53.312 | 1.00 | 25.79 |
| ATOM | 1528 | O   | ILE A 197 | 5.281  | 35.395 | 52.833 | 1.00 | 22.84 |
| ATOM | 1529 | CB  | ILE A 197 | 8.228  | 36.535 | 52.230 | 1.00 | 23.36 |
| ATOM | 1530 | CG1 | ILE A 197 | 7.164  | 37.355 | 51.526 | 1.00 | 25.01 |
| ATOM | 1531 | CG2 | ILE A 197 | 9.509  | 36.554 | 51.399 | 1.00 | 21.56 |
| ATOM | 1532 | CD1 | ILE A 197 | 7.429  | 38.859 | 51.634 | 1.00 | 22.37 |
| ATOM | 1533 | N   | PRO A 198 | 6.720  | 35.261 | 54.633 | 1.00 | 20.61 |
| ATOM | 1534 | CA  | PRO A 198 | 5.687  | 35.453 | 55.660 | 1.00 | 15.95 |
| ATOM | 1535 | C   | PRO A 198 | 5.298  | 36.916 | 55.491 | 1.00 | 17.92 |
| ATOM | 1536 | O   | PRO A 198 | 6.185  | 37.687 | 55.086 | 1.00 | 17.98 |
| ATOM | 1537 | CB  | PRO A 198 | 6.399  | 35.297 | 57.011 | 1.00 | 15.44 |
| ATOM | 1538 | CG  | PRO A 198 | 7.881  | 35.462 | 56.704 | 1.00 | 18.48 |
| ATOM | 1539 | CD  | PRO A 198 | 8.088  | 35.164 | 55.223 | 1.00 | 15.86 |
| ATOM | 1540 | N   | CYS A 199 | 4.030  | 37.325 | 55.748 | 1.00 | 18.80 |
| ATOM | 1541 | CA  | CYS A 199 | 3.646  | 38.750 | 55.529 | 1.00 | 19.91 |
| ATOM | 1542 | C   | CYS A 199 | 4.363  | 39.820 | 56.400 | 1.00 | 22.70 |
| ATOM | 1543 | O   | CYS A 199 | 4.392  | 41.030 | 56.091 | 1.00 | 19.22 |
| ATOM | 1544 | CB  | CYS A 199 | 2.118  | 38.964 | 55.554 | 1.00 | 17.27 |
| ATOM | 1545 | SG  | CYS A 199 | 1.359  | 38.495 | 57.126 | 1.00 | 22.02 |
| ATOM | 1546 | N   | TYR A 200 | 4.963  | 39.375 | 57.512 | 1.00 | 20.55 |
| ATOM | 1547 | CA  | TYR A 200 | 5.652  | 40.318 | 58.356 | 1.00 | 19.65 |
| ATOM | 1548 | C   | TYR A 200 | 6.894  | 40.879 | 57.724 | 1.00 | 24.32 |
| ATOM | 1549 | O   | TYR A 200 | 7.493  | 41.812 | 58.252 | 1.00 | 26.71 |
| ATOM | 1550 | CB  | TYR A 200 | 5.978  | 39.763 | 59.731 | 1.00 | 17.18 |
| ATOM | 1551 | CG  | TYR A 200 | 7.086  | 38.751 | 59.710 | 1.00 | 17.72 |
| ATOM | 1552 | CD1 | TYR A 200 | 8.409  | 39.169 | 59.846 | 1.00 | 16.87 |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 1553 | CD2 | TYR | A | 200 | 6.802  | 37.385 | 59.642 | 1.00 | 18.65 |
| ATOM | 1554 | CE1 | TYR | A | 200 | 9.432  | 38.221 | 59.864 | 1.00 | 14.67 |
| ATOM | 1555 | CE2 | TYR | A | 200 | 7.822  | 36.434 | 59.699 | 1.00 | 18.76 |
| ATOM | 1556 | CZ  | TYR | A | 200 | 9.146  | 36.855 | 59.802 | 1.00 | 20.42 |
| ATOM | 1557 | OH  | TYR | A | 200 | 10.169 | 35.921 | 59.858 | 1.00 | 17.42 |
| ATOM | 1558 | N   | LEU | A | 201 | 7.280  | 40.312 | 56.590 | 1.00 | 16.84 |
| ATOM | 1559 | CA  | LEU | A | 201 | 8.436  | 40.765 | 55.864 | 1.00 | 14.82 |
| ATOM | 1560 | C   | LEU | A | 201 | 8.078  | 41.787 | 54.785 | 1.00 | 24.60 |
| ATOM | 1561 | O   | LEU | A | 201 | 8.956  | 42.269 | 54.044 | 1.00 | 22.81 |
| ATOM | 1562 | CB  | LEU | A | 201 | 9.138  | 39.532 | 55.256 | 1.00 | 17.56 |
| ATOM | 1563 | CG  | LEU | A | 201 | 9.910  | 38.670 | 56.257 | 1.00 | 16.40 |
| ATOM | 1564 | CD1 | LEU | A | 201 | 10.674 | 37.594 | 55.489 | 1.00 | 15.76 |
| ATOM | 1565 | CD2 | LEU | A | 201 | 10.900 | 39.523 | 57.040 | 1.00 | 16.02 |
| ATOM | 1566 | N   | ILE | A | 202 | 6.761  | 42.084 | 54.657 | 1.00 | 24.26 |
| ATOM | 1567 | CA  | ILE | A | 202 | 6.293  | 43.088 | 53.698 | 1.00 | 20.28 |
| ATOM | 1568 | C   | ILE | A | 202 | 6.703  | 44.481 | 54.226 | 1.00 | 25.46 |
| ATOM | 1569 | O   | ILE | A | 202 | 6.447  | 44.850 | 55.393 | 1.00 | 26.48 |
| ATOM | 1570 | CB  | ILE | A | 202 | 4.784  | 43.015 | 53.489 | 1.00 | 21.23 |
| ATOM | 1571 | CG1 | ILE | A | 202 | 4.433  | 41.851 | 52.593 | 1.00 | 17.03 |
| ATOM | 1572 | CG2 | ILE | A | 202 | 4.312  | 44.312 | 52.826 | 1.00 | 23.71 |
| ATOM | 1573 | CD1 | ILE | A | 202 | 2.917  | 41.692 | 52.437 | 1.00 | 22.39 |
| ATOM | 1574 | N   | ALA | A | 203 | 7.375  | 45.252 | 53.384 | 1.00 | 17.97 |
| ATOM | 1575 | CA  | ALA | A | 203 | 7.860  | 46.568 | 53.782 | 1.00 | 22.84 |
| ATOM | 1576 | C   | ALA | A | 203 | 7.849  | 47.593 | 52.658 | 1.00 | 30.22 |
| ATOM | 1577 | O   | ALA | A | 203 | 8.125  | 47.284 | 51.494 | 1.00 | 27.07 |
| ATOM | 1578 | CB  | ALA | A | 203 | 9.284  | 46.554 | 54.360 | 1.00 | 20.04 |
| ATOM | 1579 | N   | LEU | A | 204 | 7.589  | 48.823 | 53.117 | 1.00 | 25.33 |
| ATOM | 1580 | CA  | LEU | A | 204 | 7.503  | 50.022 | 52.300 | 1.00 | 23.92 |
| ATOM | 1581 | C   | LEU | A | 204 | 8.105  | 51.242 | 53.003 | 1.00 | 27.30 |
| ATOM | 1582 | O   | LEU | A | 204 | 8.004  | 51.419 | 54.219 | 1.00 | 24.19 |
| ATOM | 1583 | CB  | LEU | A | 204 | 6.008  | 50.269 | 51.933 | 1.00 | 22.42 |
| ATOM | 1584 | CG  | LEU | A | 204 | 5.702  | 51.492 | 51.036 | 1.00 | 24.14 |
| ATOM | 1585 | CD1 | LEU | A | 204 | 6.204  | 51.374 | 49.593 | 1.00 | 17.81 |
| ATOM | 1586 | CD2 | LEU | A | 204 | 4.210  | 51.792 | 51.073 | 1.00 | 26.36 |
| ATOM | 1587 | N   | VAL | A | 205 | 8.726  | 52.078 | 52.178 | 1.00 | 26.54 |
| ATOM | 1588 | CA  | VAL | A | 205 | 9.333  | 53.346 | 52.518 | 1.00 | 25.64 |
| ATOM | 1589 | C   | VAL | A | 205 | 9.152  | 54.299 | 51.363 | 1.00 | 30.84 |
| ATOM | 1590 | O   | VAL | A | 205 | 9.382  | 53.955 | 50.204 | 1.00 | 29.34 |
| ATOM | 1591 | CB  | VAL | A | 205 | 10.827 | 53.298 | 52.785 | 1.00 | 27.61 |
| ATOM | 1592 | CG1 | VAL | A | 205 | 11.551 | 52.637 | 51.625 | 1.00 | 25.87 |
| ATOM | 1593 | CG2 | VAL | A | 205 | 11.359 | 54.717 | 53.021 | 1.00 | 27.64 |
| ATOM | 1594 | N   | VAL | A | 206 | 8.763  | 55.503 | 51.704 | 1.00 | 28.24 |
| ATOM | 1595 | CA  | VAL | A | 206 | 8.600  | 56.544 | 50.709 | 1.00 | 27.85 |
| ATOM | 1596 | C   | VAL | A | 206 | 9.246  | 57.813 | 51.206 | 1.00 | 30.43 |
| ATOM | 1597 | O   | VAL | A | 206 | 8.961  | 58.289 | 52.320 | 1.00 | 31.87 |
| ATOM | 1598 | CB  | VAL | A | 206 | 7.145  | 56.882 | 50.379 | 1.00 | 30.77 |
| ATOM | 1599 | CG1 | VAL | A | 206 | 7.113  | 57.870 | 49.200 | 1.00 | 33.19 |
| ATOM | 1600 | CG2 | VAL | A | 206 | 6.336  | 55.620 | 50.078 | 1.00 | 26.71 |
| ATOM | 1601 | N   | GLY | A | 207 | 10.098 | 58.357 | 50.363 | 1.00 | 25.40 |
| ATOM | 1602 | CA  | GLY | A | 207 | 10.706 | 59.596 | 50.760 | 1.00 | 28.31 |
| ATOM | 1603 | C   | GLY | A | 207 | 11.654 | 60.097 | 49.716 | 1.00 | 35.37 |
| ATOM | 1604 | O   | GLY | A | 207 | 11.688 | 59.549 | 48.615 | 1.00 | 34.13 |
| ATOM | 1605 | N   | ALA | A | 208 | 12.414 | 61.121 | 50.123 | 1.00 | 33.99 |
| ATOM | 1606 | CA  | ALA | A | 208 | 13.414 | 61.776 | 49.290 | 1.00 | 35.45 |
| ATOM | 1607 | C   | ALA | A | 208 | 14.746 | 61.041 | 49.360 | 1.00 | 38.58 |
| ATOM | 1608 | O   | ALA | A | 208 | 15.799 | 61.544 | 49.784 | 1.00 | 39.24 |
| ATOM | 1609 | CB  | ALA | A | 208 | 13.502 | 63.268 | 49.619 | 1.00 | 36.08 |
| ATOM | 1610 | N   | LEU | A | 209 | 14.676 | 59.796 | 48.916 | 1.00 | 34.99 |



|      |      |     |     |   |     |        |        |        |      |        |
|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
| ATOM | 1611 | CA  | LEU | A | 209 | 15.821 | 58.918 | 48.962 | 1.00 | 32.15  |
| ATOM | 1612 | C   | LEU | A | 209 | 16.730 | 59.052 | 47.800 | 1.00 | 43.00  |
| ATOM | 1613 | O   | LEU | A | 209 | 16.298 | 59.315 | 46.679 | 1.00 | 44.56  |
| ATOM | 1614 | CB  | LEU | A | 209 | 15.384 | 57.449 | 49.000 | 1.00 | 30.82  |
| ATOM | 1615 | CG  | LEU | A | 209 | 14.293 | 57.238 | 50.030 | 1.00 | 34.48  |
| ATOM | 1616 | CD1 | LEU | A | 209 | 13.712 | 55.840 | 49.875 | 1.00 | 31.95  |
| ATOM | 1617 | CD2 | LEU | A | 209 | 14.955 | 57.428 | 51.386 | 1.00 | 31.78  |
| ATOM | 1618 | N   | GLU | A | 210 | 17.979 | 58.795 | 48.156 | 1.00 | 39.96  |
| ATOM | 1619 | CA  | GLU | A | 210 | 19.130 | 58.767 | 47.294 | 1.00 | 37.51  |
| ATOM | 1620 | C   | GLU | A | 210 | 19.802 | 57.468 | 47.652 | 1.00 | 45.24  |
| ATOM | 1621 | O   | GLU | A | 210 | 19.520 | 56.916 | 48.716 | 1.00 | 45.87  |
| ATOM | 1622 | CB  | GLU | A | 210 | 20.088 | 59.940 | 47.570 | 1.00 | 39.44  |
| ATOM | 1623 | CG  | GLU | A | 210 | 19.601 | 61.256 | 46.936 | 1.00 | 43.88  |
| ATOM | 1624 | CD  | GLU | A | 210 | 20.679 | 62.289 | 46.960 | 1.00 | 83.62  |
| ATOM | 1625 | OE1 | GLU | A | 210 | 21.851 | 62.020 | 47.179 | 1.00 | 69.67  |
| ATOM | 1626 | OE2 | GLU | A | 210 | 20.217 | 63.498 | 46.755 | 1.00 | 100.00 |
| ATOM | 1627 | N   | SER | A | 211 | 20.661 | 56.973 | 46.774 | 1.00 | 39.83  |
| ATOM | 1628 | CA  | SER | A | 211 | 21.323 | 55.719 | 47.046 | 1.00 | 39.26  |
| ATOM | 1629 | C   | SER | A | 211 | 22.763 | 55.796 | 46.628 | 1.00 | 40.32  |
| ATOM | 1630 | O   | SER | A | 211 | 23.122 | 56.657 | 45.861 | 1.00 | 47.20  |
| ATOM | 1631 | CB  | SER | A | 211 | 20.662 | 54.587 | 46.273 | 1.00 | 44.16  |
| ATOM | 1632 | OG  | SER | A | 211 | 20.992 | 54.685 | 44.896 | 1.00 | 48.01  |
| ATOM | 1633 | N   | ARG | A | 212 | 23.589 | 54.915 | 47.123 | 1.00 | 30.46  |
| ATOM | 1634 | CA  | ARG | A | 212 | 24.981 | 54.860 | 46.737 | 1.00 | 30.14  |
| ATOM | 1635 | C   | ARG | A | 212 | 25.200 | 53.371 | 46.539 | 1.00 | 38.14  |
| ATOM | 1636 | O   | ARG | A | 212 | 24.617 | 52.557 | 47.252 | 1.00 | 38.33  |
| ATOM | 1637 | CB  | ARG | A | 212 | 25.928 | 55.449 | 47.785 | 1.00 | 36.60  |
| ATOM | 1638 | CG  | ARG | A | 212 | 26.973 | 56.473 | 47.307 | 1.00 | 66.52  |
| ATOM | 1639 | CD  | ARG | A | 212 | 26.437 | 57.592 | 46.403 | 1.00 | 92.22  |
| ATOM | 1640 | NE  | ARG | A | 212 | 26.336 | 58.944 | 46.974 | 1.00 | 88.06  |
| ATOM | 1641 | CZ  | ARG | A | 212 | 25.429 | 59.863 | 46.586 | 1.00 | 100.00 |
| ATOM | 1642 | NH1 | ARG | A | 212 | 24.525 | 59.616 | 45.636 | 1.00 | 63.09  |
| ATOM | 1643 | NH2 | ARG | A | 212 | 25.405 | 61.069 | 47.169 | 1.00 | 100.00 |
| ATOM | 1644 | N   | GLN | A | 213 | 25.985 | 52.957 | 45.570 | 1.00 | 34.56  |
| ATOM | 1645 | CA  | GLN | A | 213 | 26.155 | 51.533 | 45.435 | 1.00 | 34.71  |
| ATOM | 1646 | C   | GLN | A | 213 | 27.453 | 51.142 | 46.101 | 1.00 | 40.21  |
| ATOM | 1647 | O   | GLN | A | 213 | 28.493 | 51.737 | 45.826 | 1.00 | 41.35  |
| ATOM | 1648 | CB  | GLN | A | 213 | 26.081 | 51.014 | 44.000 | 1.00 | 36.31  |
| ATOM | 1649 | CG  | GLN | A | 213 | 26.626 | 49.582 | 43.946 | 1.00 | 49.64  |
| ATOM | 1650 | CD  | GLN | A | 213 | 26.775 | 49.077 | 42.531 | 1.00 | 80.06  |
| ATOM | 1651 | OE1 | GLN | A | 213 | 26.908 | 47.861 | 42.312 | 1.00 | 77.10  |
| ATOM | 1652 | NE2 | GLN | A | 213 | 26.753 | 50.012 | 41.577 | 1.00 | 75.51  |
| ATOM | 1653 | N   | ILE | A | 214 | 27.370 | 50.166 | 47.007 | 1.00 | 35.56  |
| ATOM | 1654 | CA  | ILE | A | 214 | 28.531 | 49.737 | 47.760 | 1.00 | 32.74  |
| ATOM | 1655 | C   | ILE | A | 214 | 28.947 | 48.311 | 47.535 | 1.00 | 28.86  |
| ATOM | 1656 | O   | ILE | A | 214 | 29.917 | 47.897 | 48.149 | 1.00 | 30.02  |
| ATOM | 1657 | CB  | ILE | A | 214 | 28.320 | 49.957 | 49.262 | 1.00 | 39.00  |
| ATOM | 1658 | CG1 | ILE | A | 214 | 27.032 | 49.265 | 49.733 | 1.00 | 40.79  |
| ATOM | 1659 | CG2 | ILE | A | 214 | 28.198 | 51.447 | 49.566 | 1.00 | 39.90  |
| ATOM | 1660 | CD1 | ILE | A | 214 | 26.810 | 49.364 | 51.247 | 1.00 | 39.31  |
| ATOM | 1661 | N   | GLY | A | 215 | 28.231 | 47.569 | 46.691 | 1.00 | 29.42  |
| ATOM | 1662 | CA  | GLY | A | 215 | 28.518 | 46.166 | 46.367 | 1.00 | 26.41  |
| ATOM | 1663 | C   | GLY | A | 215 | 27.778 | 45.743 | 45.106 | 1.00 | 30.00  |
| ATOM | 1664 | O   | GLY | A | 215 | 26.874 | 46.447 | 44.669 | 1.00 | 35.16  |
| ATOM | 1665 | N   | PRO | A | 216 | 28.131 | 44.608 | 44.497 | 1.00 | 33.24  |
| ATOM | 1666 | CA  | PRO | A | 216 | 27.459 | 44.197 | 43.262 | 1.00 | 33.84  |
| ATOM | 1667 | C   | PRO | A | 216 | 25.979 | 43.984 | 43.441 | 1.00 | 39.13  |
| ATOM | 1668 | O   | PRO | A | 216 | 25.241 | 44.145 | 42.467 | 1.00 | 40.02  |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 1669 | CB  | PRO | A | 216 | 28.067 | 42.867 | 42.793 | 1.00 | 34.78 |
| ATOM | 1670 | CG  | PRO | A | 216 | 29.020 | 42.415 | 43.897 | 1.00 | 38.44 |
| ATOM | 1671 | CD  | PRO | A | 216 | 29.116 | 43.556 | 44.912 | 1.00 | 35.07 |
| ATOM | 1672 | N   | ARG | A | 217 | 25.578 | 43.609 | 44.662 | 1.00 | 23.56 |
| ATOM | 1673 | CA  | ARG | A | 217 | 24.177 | 43.370 | 44.909 | 1.00 | 21.48 |
| ATOM | 1674 | C   | ARG | A | 217 | 23.679 | 44.288 | 46.015 | 1.00 | 30.90 |
| ATOM | 1675 | O   | ARG | A | 217 | 22.706 | 44.002 | 46.713 | 1.00 | 27.14 |
| ATOM | 1676 | CB  | ARG | A | 217 | 23.926 | 41.920 | 45.247 | 1.00 | 22.22 |
| ATOM | 1677 | CG  | ARG | A | 217 | 25.122 | 41.312 | 45.977 | 1.00 | 30.92 |
| ATOM | 1678 | CD  | ARG | A | 217 | 24.882 | 39.839 | 46.242 | 1.00 | 25.36 |
| ATOM | 1679 | NE  | ARG | A | 217 | 26.009 | 39.174 | 46.874 | 1.00 | 30.74 |
| ATOM | 1680 | CZ  | ARG | A | 217 | 26.020 | 37.875 | 47.141 | 1.00 | 32.19 |
| ATOM | 1681 | NH1 | ARG | A | 217 | 24.991 | 37.088 | 46.838 | 1.00 | 29.57 |
| ATOM | 1682 | NH2 | ARG | A | 217 | 27.090 | 37.341 | 47.732 | 1.00 | 42.93 |
| ATOM | 1683 | N   | THR | A | 218 | 24.354 | 45.426 | 46.134 | 1.00 | 27.52 |
| ATOM | 1684 | CA  | THR | A | 218 | 23.979 | 46.331 | 47.172 | 1.00 | 25.01 |
| ATOM | 1685 | C   | THR | A | 218 | 24.154 | 47.813 | 46.936 | 1.00 | 29.25 |
| ATOM | 1686 | O   | THR | A | 218 | 25.256 | 48.269 | 46.674 | 1.00 | 32.56 |
| ATOM | 1687 | CB  | THR | A | 218 | 24.877 | 46.003 | 48.388 | 1.00 | 30.92 |
| ATOM | 1688 | OG1 | THR | A | 218 | 24.591 | 44.711 | 48.891 | 1.00 | 28.41 |
| ATOM | 1689 | CG2 | THR | A | 218 | 24.710 | 47.060 | 49.474 | 1.00 | 27.73 |
| ATOM | 1690 | N   | LEU | A | 219 | 23.056 | 48.543 | 47.133 | 1.00 | 25.49 |
| ATOM | 1691 | CA  | LEU | A | 219 | 22.997 | 49.991 | 47.132 | 1.00 | 27.09 |
| ATOM | 1692 | C   | LEU | A | 219 | 22.572 | 50.417 | 48.532 | 1.00 | 35.31 |
| ATOM | 1693 | O   | LEU | A | 219 | 21.748 | 49.739 | 49.162 | 1.00 | 32.55 |
| ATOM | 1694 | CB  | LEU | A | 219 | 21.822 | 50.526 | 46.319 | 1.00 | 29.51 |
| ATOM | 1695 | CG  | LEU | A | 219 | 22.159 | 50.812 | 44.869 | 1.00 | 31.54 |
| ATOM | 1696 | CD1 | LEU | A | 219 | 23.162 | 49.773 | 44.395 | 1.00 | 31.76 |
| ATOM | 1697 | CD2 | LEU | A | 219 | 20.836 | 50.658 | 44.148 | 1.00 | 32.31 |
| ATOM | 1698 | N   | VAL | A | 220 | 23.086 | 51.549 | 49.001 | 1.00 | 31.15 |
| ATOM | 1699 | CA  | VAL | A | 220 | 22.715 | 52.101 | 50.289 | 1.00 | 31.32 |
| ATOM | 1700 | C   | VAL | A | 220 | 21.720 | 53.197 | 50.002 | 1.00 | 31.45 |
| ATOM | 1701 | O   | VAL | A | 220 | 22.004 | 54.072 | 49.190 | 1.00 | 31.85 |
| ATOM | 1702 | CB  | VAL | A | 220 | 23.878 | 52.729 | 51.089 | 1.00 | 39.68 |
| ATOM | 1703 | CG1 | VAL | A | 220 | 23.538 | 52.833 | 52.574 | 1.00 | 37.81 |
| ATOM | 1704 | CG2 | VAL | A | 220 | 25.193 | 51.970 | 50.965 | 1.00 | 42.41 |
| ATOM | 1705 | N   | TRP | A | 221 | 20.579 | 53.168 | 50.665 | 1.00 | 28.89 |
| ATOM | 1706 | CA  | TRP | A | 221 | 19.574 | 54.197 | 50.471 | 1.00 | 30.76 |
| ATOM | 1707 | C   | TRP | A | 221 | 19.317 | 55.010 | 51.729 | 1.00 | 38.31 |
| ATOM | 1708 | O   | TRP | A | 221 | 19.205 | 54.446 | 52.812 | 1.00 | 35.62 |
| ATOM | 1709 | CB  | TRP | A | 221 | 18.240 | 53.555 | 50.116 | 1.00 | 30.66 |
| ATOM | 1710 | CG  | TRP | A | 221 | 18.321 | 52.711 | 48.896 | 1.00 | 34.85 |
| ATOM | 1711 | CD1 | TRP | A | 221 | 18.752 | 51.434 | 48.798 | 1.00 | 37.00 |
| ATOM | 1712 | CD2 | TRP | A | 221 | 17.952 | 53.129 | 47.584 | 1.00 | 36.50 |
| ATOM | 1713 | NE1 | TRP | A | 221 | 18.648 | 51.014 | 47.501 | 1.00 | 35.82 |
| ATOM | 1714 | CE2 | TRP | A | 221 | 18.154 | 52.033 | 46.737 | 1.00 | 39.42 |
| ATOM | 1715 | CE3 | TRP | A | 221 | 17.429 | 54.325 | 47.067 | 1.00 | 36.65 |
| ATOM | 1716 | CZ2 | TRP | A | 221 | 17.864 | 52.123 | 45.374 | 1.00 | 38.93 |
| ATOM | 1717 | CZ3 | TRP | A | 221 | 17.124 | 54.398 | 45.732 | 1.00 | 36.06 |
| ATOM | 1718 | CH2 | TRP | A | 221 | 17.353 | 53.308 | 44.897 | 1.00 | 36.29 |
| ATOM | 1719 | N   | SER | A | 222 | 19.172 | 56.319 | 51.557 | 1.00 | 31.91 |
| ATOM | 1720 | CA  | SER | A | 222 | 18.877 | 57.235 | 52.639 | 1.00 | 32.45 |
| ATOM | 1721 | C   | SER | A | 222 | 18.692 | 58.639 | 52.086 | 1.00 | 40.59 |
| ATOM | 1722 | O   | SER | A | 222 | 18.918 | 58.901 | 50.894 | 1.00 | 40.28 |
| ATOM | 1723 | CB  | SER | A | 222 | 19.941 | 57.242 | 53.735 | 1.00 | 31.75 |
| ATOM | 1724 | OG  | SER | A | 222 | 21.077 | 57.977 | 53.297 | 1.00 | 35.91 |
| ATOM | 1725 | N   | GLU | A | 223 | 18.277 | 59.534 | 52.972 | 1.00 | 31.05 |
| ATOM | 1726 | CA  | GLU | A | 223 | 18.173 | 60.885 | 52.539 | 1.00 | 28.81 |



|      |      |     |     |   |     |        |        |        |      |        |
|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
| ATOM | 1727 | C   | GLU | A | 223 | 19.612 | 61.239 | 52.186 | 1.00 | 38.65  |
| ATOM | 1728 | O   | GLU | A | 223 | 20.566 | 60.582 | 52.608 | 1.00 | 34.90  |
| ATOM | 1729 | CB  | GLU | A | 223 | 17.638 | 61.815 | 53.630 | 1.00 | 27.66  |
| ATOM | 1730 | CG  | GLU | A | 223 | 16.099 | 61.840 | 53.673 | 1.00 | 36.07  |
| ATOM | 1731 | CD  | GLU | A | 223 | 15.540 | 62.978 | 54.497 | 1.00 | 57.21  |
| ATOM | 1732 | OE1 | GLU | A | 223 | 15.442 | 64.108 | 54.071 | 1.00 | 40.65  |
| ATOM | 1733 | OE2 | GLU | A | 223 | 15.155 | 62.645 | 55.711 | 1.00 | 38.93  |
| ATOM | 1734 | N   | LYS | A | 224 | 19.740 | 62.273 | 51.372 | 1.00 | 39.48  |
| ATOM | 1735 | CA  | LYS | A | 224 | 20.983 | 62.809 | 50.871 | 1.00 | 37.65  |
| ATOM | 1736 | C   | LYS | A | 224 | 22.045 | 62.999 | 51.962 | 1.00 | 35.43  |
| ATOM | 1737 | O   | LYS | A | 224 | 23.215 | 62.614 | 51.833 | 1.00 | 35.56  |
| ATOM | 1738 | CB  | LYS | A | 224 | 20.645 | 64.109 | 50.115 | 1.00 | 39.12  |
| ATOM | 1739 | CG  | LYS | A | 224 | 21.806 | 64.741 | 49.359 | 1.00 | 73.65  |
| ATOM | 1740 | CD  | LYS | A | 224 | 21.391 | 65.942 | 48.513 | 1.00 | 100.00 |
| ATOM | 1741 | CE  | LYS | A | 224 | 21.854 | 67.295 | 49.055 | 1.00 | 100.00 |
| ATOM | 1742 | NZ  | LYS | A | 224 | 21.228 | 68.446 | 48.366 | 1.00 | 100.00 |
| ATOM | 1743 | N   | GLU | A | 225 | 21.631 | 63.614 | 53.061 | 1.00 | 29.04  |
| ATOM | 1744 | CA  | GLU | A | 225 | 22.503 | 63.910 | 54.177 | 1.00 | 29.49  |
| ATOM | 1745 | C   | GLU | A | 225 | 23.114 | 62.705 | 54.868 | 1.00 | 38.42  |
| ATOM | 1746 | O   | GLU | A | 225 | 24.074 | 62.857 | 55.612 | 1.00 | 41.35  |
| ATOM | 1747 | CB  | GLU | A | 225 | 21.760 | 64.741 | 55.223 | 1.00 | 32.49  |
| ATOM | 1748 | CG  | GLU | A | 225 | 20.251 | 64.516 | 55.075 | 1.00 | 59.17  |
| ATOM | 1749 | CD  | GLU | A | 225 | 19.687 | 65.377 | 53.982 | 1.00 | 72.33  |
| ATOM | 1750 | OE1 | GLU | A | 225 | 20.013 | 66.539 | 53.851 | 1.00 | 51.07  |
| ATOM | 1751 | OE2 | GLU | A | 225 | 18.840 | 64.757 | 53.195 | 1.00 | 54.65  |
| ATOM | 1752 | N   | GLN | A | 226 | 22.575 | 61.511 | 54.647 | 1.00 | 36.99  |
| ATOM | 1753 | CA  | GLN | A | 226 | 23.114 | 60.333 | 55.307 | 1.00 | 33.80  |
| ATOM | 1754 | C   | GLN | A | 226 | 23.845 | 59.389 | 54.379 | 1.00 | 32.45  |
| ATOM | 1755 | O   | GLN | A | 226 | 24.549 | 58.487 | 54.812 | 1.00 | 29.61  |
| ATOM | 1756 | CB  | GLN | A | 226 | 21.953 | 59.585 | 55.988 | 1.00 | 33.92  |
| ATOM | 1757 | CG  | GLN | A | 226 | 21.625 | 60.145 | 57.379 | 1.00 | 27.50  |
| ATOM | 1758 | CD  | GLN | A | 226 | 21.179 | 61.600 | 57.359 | 1.00 | 47.10  |
| ATOM | 1759 | OE1 | GLN | A | 226 | 21.839 | 62.495 | 57.933 | 1.00 | 40.63  |
| ATOM | 1760 | NE2 | GLN | A | 226 | 20.042 | 61.842 | 56.717 | 1.00 | 26.24  |
| ATOM | 1761 | N   | VAL | A | 227 | 23.678 | 59.591 | 53.084 | 1.00 | 33.73  |
| ATOM | 1762 | CA  | VAL | A | 227 | 24.256 | 58.708 | 52.072 | 1.00 | 36.03  |
| ATOM | 1763 | C   | VAL | A | 227 | 25.733 | 58.366 | 52.155 | 1.00 | 38.24  |
| ATOM | 1764 | O   | VAL | A | 227 | 26.180 | 57.209 | 52.105 | 1.00 | 36.89  |
| ATOM | 1765 | CB  | VAL | A | 227 | 23.935 | 59.160 | 50.648 | 1.00 | 41.90  |
| ATOM | 1766 | CG1 | VAL | A | 227 | 25.168 | 58.940 | 49.784 | 1.00 | 41.75  |
| ATOM | 1767 | CG2 | VAL | A | 227 | 22.767 | 58.374 | 50.066 | 1.00 | 41.36  |
| ATOM | 1768 | N   | GLU | A | 228 | 26.504 | 59.419 | 52.206 | 1.00 | 29.72  |
| ATOM | 1769 | CA  | GLU |   |     |        |        |        |      |        |



|      |      |     |     |   |     |        |        |        |            |
|------|------|-----|-----|---|-----|--------|--------|--------|------------|
| ATOM | 1785 | NZ  | LYS | A | 229 | 30.083 | 60.097 | 61.477 | 1.00100.00 |
| ATOM | 1786 | N   | SER | A | 230 | 26.660 | 56.593 | 55.349 | 1.00 23.52 |
| ATOM | 1787 | CA  | SER | A | 230 | 26.178 | 55.239 | 55.340 | 1.00 22.02 |
| ATOM | 1788 | C   | SER | A | 230 | 27.057 | 54.388 | 54.459 | 1.00 28.88 |
| ATOM | 1789 | O   | SER | A | 230 | 27.446 | 53.270 | 54.798 | 1.00 26.72 |
| ATOM | 1790 | CB  | SER | A | 230 | 24.794 | 55.259 | 54.768 | 1.00 24.16 |
| ATOM | 1791 | OG  | SER | A | 230 | 23.976 | 55.991 | 55.660 | 1.00 31.92 |
| ATOM | 1792 | N   | ALA | A | 231 | 27.338 | 54.956 | 53.295 | 1.00 30.71 |
| ATOM | 1793 | CA  | ALA | A | 231 | 28.162 | 54.287 | 52.314 | 1.00 31.57 |
| ATOM | 1794 | C   | ALA | A | 231 | 29.460 | 53.827 | 52.957 | 1.00 35.46 |
| ATOM | 1795 | O   | ALA | A | 231 | 29.919 | 52.702 | 52.752 | 1.00 38.54 |
| ATOM | 1796 | CB  | ALA | A | 231 | 28.363 | 55.167 | 51.087 | 1.00 31.57 |
| ATOM | 1797 | N   | TYR | A | 232 | 30.052 | 54.699 | 53.773 | 1.00 32.67 |
| ATOM | 1798 | CA  | TYR | A | 232 | 31.271 | 54.323 | 54.472 | 1.00 30.97 |
| ATOM | 1799 | C   | TYR | A | 232 | 31.016 | 53.245 | 55.541 | 1.00 31.41 |
| ATOM | 1800 | O   | TYR | A | 232 | 31.694 | 52.206 | 55.613 | 1.00 25.59 |
| ATOM | 1801 | CB  | TYR | A | 232 | 31.896 | 55.533 | 55.199 | 1.00 31.17 |
| ATOM | 1802 | CG  | TYR | A | 232 | 33.004 | 55.084 | 56.136 | 1.00 36.66 |
| ATOM | 1803 | CD1 | TYR | A | 232 | 34.306 | 54.872 | 55.667 | 1.00 38.45 |
| ATOM | 1804 | CD2 | TYR | A | 232 | 32.744 | 54.825 | 57.484 | 1.00 38.25 |
| ATOM | 1805 | CE1 | TYR | A | 232 | 35.336 | 54.432 | 56.501 | 1.00 38.86 |
| ATOM | 1806 | CE2 | TYR | A | 232 | 33.761 | 54.375 | 58.332 | 1.00 40.20 |
| ATOM | 1807 | CZ  | TYR | A | 232 | 35.054 | 54.174 | 57.844 | 1.00 53.86 |
| ATOM | 1808 | OH  | TYR | A | 232 | 36.048 | 53.741 | 58.690 | 1.00 61.49 |
| ATOM | 1809 | N   | GLU | A | 233 | 30.031 | 53.541 | 56.397 | 1.00 25.55 |
| ATOM | 1810 | CA  | GLU | A | 233 | 29.707 | 52.671 | 57.515 | 1.00 26.18 |
| ATOM | 1811 | C   | GLU | A | 233 | 29.512 | 51.180 | 57.188 | 1.00 29.28 |
| ATOM | 1812 | O   | GLU | A | 233 | 29.995 | 50.286 | 57.894 | 1.00 24.42 |
| ATOM | 1813 | CB  | GLU | A | 233 | 28.552 | 53.249 | 58.378 | 1.00 25.67 |
| ATOM | 1814 | CG  | GLU | A | 233 | 28.555 | 52.694 | 59.834 | 1.00 18.89 |
| ATOM | 1815 | CD  | GLU | A | 233 | 29.382 | 53.550 | 60.760 | 1.00 26.93 |
| ATOM | 1816 | OE1 | GLU | A | 233 | 29.452 | 54.765 | 60.620 | 1.00 27.88 |
| ATOM | 1817 | OE2 | GLU | A | 233 | 30.040 | 52.884 | 61.693 | 1.00 24.94 |
| ATOM | 1818 | N   | PHE | A | 234 | 28.771 | 50.928 | 56.103 | 1.00 24.06 |
| ATOM | 1819 | CA  | PHE | A | 234 | 28.405 | 49.601 | 55.690 | 1.00 21.98 |
| ATOM | 1820 | C   | PHE | A | 234 | 29.236 | 48.989 | 54.590 | 1.00 28.86 |
| ATOM | 1821 | O   | PHE | A | 234 | 28.824 | 48.018 | 53.970 | 1.00 31.83 |
| ATOM | 1822 | CB  | PHE | A | 234 | 26.896 | 49.559 | 55.393 | 1.00 24.08 |
| ATOM | 1823 | CG  | PHE | A | 234 | 26.104 | 50.243 | 56.504 | 1.00 26.00 |
| ATOM | 1824 | CD1 | PHE | A | 234 | 26.254 | 49.860 | 57.840 | 1.00 25.17 |
| ATOM | 1825 | CD2 | PHE | A | 234 | 25.221 | 51.293 | 56.243 | 1.00 24.04 |
| ATOM | 1826 | CE1 | PHE | A | 234 | 25.543 | 50.470 | 58.875 | 1.00 22.99 |
| ATOM | 1827 | CE2 | PHE | A | 234 | 24.510 | 51.932 | 57.263 | 1.00 27.32 |
| ATOM | 1828 | CZ  | PHE | A | 234 | 24.676 | 51.524 | 58.588 | 1.00 21.69 |
| ATOM | 1829 | N   | SER | A | 235 | 30.404 | 49.560 | 54.355 | 1.00 26.37 |
| ATOM | 1830 | CA  | SER | A | 235 | 31.316 | 49.070 | 53.330 | 1.00 23.42 |
| ATOM | 1831 | C   | SER | A | 235 | 31.477 | 47.546 | 53.325 | 1.00 29.66 |
| ATOM | 1832 | O   | SER | A | 235 | 31.561 | 46.923 | 52.270 | 1.00 28.78 |
| ATOM | 1833 | CB  | SER | A | 235 | 32.649 | 49.751 | 53.541 | 1.00 21.15 |
| ATOM | 1834 | OG  | SER | A | 235 | 33.483 | 48.977 | 54.386 | 1.00 30.93 |
| ATOM | 1835 | N   | GLU | A | 236 | 31.514 | 46.917 | 54.506 | 1.00 26.42 |
| ATOM | 1836 | CA  | GLU | A | 236 | 31.708 | 45.477 | 54.600 | 1.00 24.96 |
| ATOM | 1837 | C   | GLU | A | 236 | 30.566 | 44.562 | 54.193 | 1.00 25.09 |
| ATOM | 1838 | O   | GLU | A | 236 | 30.719 | 43.346 | 54.196 | 1.00 24.51 |
| ATOM | 1839 | CB  | GLU | A | 236 | 32.243 | 45.007 | 55.968 | 1.00 27.28 |
| ATOM | 1840 | CG  | GLU | A | 236 | 33.391 | 45.867 | 56.539 | 1.00 29.83 |
| ATOM | 1841 | CD  | GLU | A | 236 | 33.396 | 45.909 | 58.055 | 1.00 62.44 |
| ATOM | 1842 | OE1 | GLU | A | 236 | 32.410 | 46.157 | 58.739 | 1.00 33.13 |



|      |      |     |     |   |     |          |        |        |      |       |
|------|------|-----|-----|---|-----|----------|--------|--------|------|-------|
| ATOM | 1843 | OE2 | GLU | A | 236 | 34.574   | 45.665 | 58.572 | 1.00 | 45.68 |
| ATOM | 1844 | N   | THR | A | 237 | 29.428   | 45.112 | 53.843 | 1.00 | 20.37 |
| ATOM | 1845 | CA  | THR | A | 237 | 28.298   | 44.271 | 53.487 | 1.00 | 20.82 |
| ATOM | 1846 | C   | THR | A | 237 | 28.534   | 43.130 | 52.541 | 1.00 | 29.25 |
| ATOM | 1847 | O   | THR | A | 237 | 28.150   | 42.007 | 52.817 | 1.00 | 32.13 |
| ATOM | 1848 | CB  | THR | A | 237 | 27.137   | 45.128 | 52.989 | 1.00 | 27.71 |
| ATOM | 1849 | OG1 | THR | A | 237 | 26.840   | 46.044 | 54.020 | 1.00 | 30.30 |
| ATOM | 1850 | CG2 | THR | A | 237 | 25.909   | 44.303 | 52.610 | 1.00 | 21.64 |
| ATOM | 1851 | N   | GLU | A | 238 | 29.126   | 43.411 | 51.399 | 1.00 | 26.94 |
| ATOM | 1852 | CA  | GLU | A | 238 | 29.306   | 42.335 | 50.454 | 1.00 | 27.77 |
| ATOM | 1853 | C   | GLU | A | 238 | 30.150   | 41.241 | 51.009 | 1.00 | 26.72 |
| ATOM | 1854 | O   | GLU | A | 238 | 29.896   | 40.077 | 50.782 | 1.00 | 32.69 |
| ATOM | 1855 | CB  | GLU | A | 238 | 29.844   | 42.795 | 49.088 | 1.00 | 28.58 |
| ATOM | 1856 | CG  | GLU | A | 238 | 30.088   | 41.593 | 48.154 | 1.00 | 27.86 |
| ATOM | 1857 | CD  | GLU | A | 238 | 28.859   | 40.827 | 47.718 | 1.00 | 21.53 |
| ATOM | 1858 | OE1 | GLU | A | 238 | 27.709   | 41.240 | 47.709 | 1.00 | 31.37 |
| ATOM | 1859 | OE2 | GLU | A | 238 | 29.193   | 39.652 | 47.262 | 1.00 | 28.77 |
| ATOM | 1860 | N   | SER | A | 239 | 31.179   | 41.605 | 51.727 | 1.00 | 21.43 |
| ATOM | 1861 | CA  | SER | A | 239 | 32.002   | 40.540 | 52.279 | 1.00 | 20.35 |
| ATOM | 1862 | C   | SER | A | 239 | 31.235   | 39.691 | 53.270 | 1.00 | 27.26 |
| ATOM | 1863 | O   | SER | A | 239 | 31.524   | 38.499 | 53.482 | 1.00 | 24.57 |
| ATOM | 1864 | CB  | SER | A | 239 | 33.268   | 41.078 | 52.951 | 1.00 | 28.19 |
| ATOM | 1865 | OG  | SER | A | 239 | 32.986   | 41.780 | 54.157 | 1.00 | 38.57 |
| ATOM | 1866 | N   | MET | A | 240 | 30.240   | 40.330 | 53.910 | 1.00 | 26.94 |
| ATOM | 1867 | CA  | MET | A | 240 | 29.432   | 39.610 | 54.898 | 1.00 | 20.31 |
| ATOM | 1868 | C   | MET | A | 240 | 28.541   | 38.616 | 54.210 | 1.00 | 17.27 |
| ATOM | 1869 | O   | MET | A | 240 | 28.413   | 37.482 | 54.657 | 1.00 | 19.98 |
| ATOM | 1870 | CB  | MET | A | 240 | 28.609   | 40.545 | 55.802 | 1.00 | 20.22 |
| ATOM | 1871 | CG  | MET | A | 240 | 29.543   | 41.286 | 56.744 | 1.00 | 21.15 |
| ATOM | 1872 | SD  | MET | A | 240 | 28.696   | 42.501 | 57.783 | 1.00 | 24.45 |
| ATOM | 1873 | CE  | MET | A | 240 | 29.842   | 42.552 | 59.180 | 1.00 | 22.66 |
| ATOM | 1874 | N   | LEU | A | 241 | 27.958   | 39.073 | 53.114 | 1.00 | 21.32 |
| ATOM | 1875 | CA  | LEU | A | 241 | 27.070   | 38.293 | 52.255 | 1.00 | 24.19 |
| ATOM | 1876 | C   | LEU | A | 241 | 27.822   | 37.062 | 51.812 | 1.00 | 27.53 |
| ATOM | 1877 | O   | LEU | A | 241 | 27.328   | 35.950 | 51.882 | 1.00 | 29.31 |
| ATOM | 1878 | CB  | LEU | A | 241 | 26.656   | 39.080 | 50.991 | 1.00 | 25.13 |
| ATOM | 1879 | CG  | LEU | A | 241 | 25.493   | 40.037 | 51.219 | 1.00 | 30.35 |
| ATOM | 1880 | CD1 | LEU | A | 241 | 25.400   | 41.089 | 50.119 | 1.00 | 27.92 |
| ATOM | 1881 | CD2 | LEU | A | 241 | 24.213   | 39.220 | 51.277 | 1.00 | 33.53 |
| ATOM | 1882 | N   | LYS | A | 242 | 29.060   | 37.257 | 51.378 | 1.00 | 25.05 |
| ATOM | 1883 | CA  | LYS | A | 242 | 29.822   | 36.095 | 50.972 | 1.00 | 23.44 |
| ATOM | 1884 | C   | LYS | A | 242 | 30.013   | 35.091 | 52.100 | 1.00 | 24.02 |
| ATOM | 1885 | O   | LYS | A | 242 | 29.895</ |        |        |      |       |



|      |      |     |     |       |        |        |        |      |       |
|------|------|-----|-----|-------|--------|--------|--------|------|-------|
| ATOM | 1901 | C   | ALA | A 244 | 26.500 | 32.902 | 53.995 | 1.00 | 29.00 |
| ATOM | 1902 | O   | ALA | A 244 | 25.878 | 31.893 | 54.323 | 1.00 | 28.18 |
| ATOM | 1903 | CB  | ALA | A 244 | 25.901 | 35.157 | 55.072 | 1.00 | 21.72 |
| ATOM | 1904 | N   | GLU | A 245 | 26.892 | 33.104 | 52.731 | 1.00 | 27.16 |
| ATOM | 1905 | CA  | GLU | A 245 | 26.581 | 32.130 | 51.706 | 1.00 | 22.70 |
| ATOM | 1906 | C   | GLU | A 245 | 27.328 | 30.874 | 52.001 | 1.00 | 25.30 |
| ATOM | 1907 | O   | GLU | A 245 | 26.844 | 29.762 | 51.887 | 1.00 | 28.85 |
| ATOM | 1908 | CB  | GLU | A 245 | 26.915 | 32.653 | 50.315 | 1.00 | 22.34 |
| ATOM | 1909 | CG  | GLU | A 245 | 25.838 | 33.625 | 49.841 | 1.00 | 26.07 |
| ATOM | 1910 | CD  | GLU | A 245 | 26.137 | 34.180 | 48.472 | 1.00 | 52.41 |
| ATOM | 1911 | OE1 | GLU | A 245 | 27.101 | 34.897 | 48.236 | 1.00 | 39.38 |
| ATOM | 1912 | OE2 | GLU | A 245 | 25.260 | 33.798 | 47.566 | 1.00 | 37.85 |
| ATOM | 1913 | N   | ASP | A 246 | 28.540 | 31.079 | 52.445 | 1.00 | 27.12 |
| ATOM | 1914 | CA  | ASP | A 246 | 29.361 | 29.946 | 52.792 | 1.00 | 29.38 |
| ATOM | 1915 | C   | ASP | A 246 | 28.782 | 29.251 | 53.996 | 1.00 | 27.88 |
| ATOM | 1916 | O   | ASP | A 246 | 28.832 | 28.037 | 54.170 | 1.00 | 23.60 |
| ATOM | 1917 | CB  | ASP | A 246 | 30.857 | 30.287 | 53.015 | 1.00 | 34.30 |
| ATOM | 1918 | CG  | ASP | A 246 | 31.627 | 29.070 | 53.420 | 1.00 | 63.22 |
| ATOM | 1919 | OD1 | ASP | A 246 | 31.877 | 28.135 | 52.678 | 1.00 | 70.56 |
| ATOM | 1920 | OD2 | ASP | A 246 | 31.934 | 29.082 | 54.686 | 1.00 | 89.74 |
| ATOM | 1921 | N   | LEU | A 247 | 28.191 | 30.025 | 54.861 | 1.00 | 22.96 |
| ATOM | 1922 | CA  | LEU | A 247 | 27.644 | 29.333 | 56.028 | 1.00 | 26.75 |
| ATOM | 1923 | C   | LEU | A 247 | 26.274 | 28.715 | 55.782 | 1.00 | 25.45 |
| ATOM | 1924 | O   | LEU | A 247 | 25.966 | 27.625 | 56.268 | 1.00 | 26.16 |
| ATOM | 1925 | CB  | LEU | A 247 | 27.522 | 30.296 | 57.251 | 1.00 | 28.55 |
| ATOM | 1926 | CG  | LEU | A 247 | 28.834 | 30.551 | 58.009 | 1.00 | 35.08 |
| ATOM | 1927 | CD1 | LEU | A 247 | 30.008 | 30.474 | 57.061 | 1.00 | 37.19 |
| ATOM | 1928 | CD2 | LEU | A 247 | 28.799 | 31.948 | 58.597 | 1.00 | 33.92 |
| ATOM | 1929 | N   | GLY | A 248 | 25.401 | 29.437 | 55.086 | 1.00 | 21.51 |
| ATOM | 1930 | CA  | GLY | A 248 | 24.075 | 28.880 | 54.940 | 1.00 | 22.31 |
| ATOM | 1931 | C   | GLY | A 248 | 23.729 | 28.415 | 53.550 | 1.00 | 28.05 |
| ATOM | 1932 | O   | GLY | A 248 | 22.623 | 27.946 | 53.306 | 1.00 | 27.83 |
| ATOM | 1933 | N   | GLY | A 249 | 24.657 | 28.534 | 52.622 | 1.00 | 23.33 |
| ATOM | 1934 | CA  | GLY | A 249 | 24.262 | 28.120 | 51.289 | 1.00 | 21.34 |
| ATOM | 1935 | C   | GLY | A 249 | 23.976 | 29.381 | 50.493 | 1.00 | 30.63 |
| ATOM | 1936 | O   | GLY | A 249 | 24.178 | 30.490 | 50.960 | 1.00 | 30.72 |
| ATOM | 1937 | N   | PRO | A 250 | 23.527 | 29.227 | 49.262 | 1.00 | 37.05 |
| ATOM | 1938 | CA  | PRO | A 250 | 23.264 | 30.361 | 48.403 | 1.00 | 37.47 |
| ATOM | 1939 | C   | PRO | A 250 | 22.230 | 31.367 | 48.883 | 1.00 | 35.89 |
| ATOM | 1940 | O   | PRO | A 250 | 21.184 | 31.002 | 49.410 | 1.00 | 32.74 |
| ATOM | 1941 | CB  | PRO | A 250 | 22.704 | 29.749 | 47.114 | 1.00 | 41.49 |
| ATOM | 1942 | CG  | PRO | A 250 | 22.260 | 28.330 | 47.442 | 1.00 | 47.11 |
| ATOM | 1943 | CD  | PRO | A 250 | 22.942 | 27.959 | 48.743 | 1.00 | 40.92 |
| ATOM | 1944 | N   | TYR | A 251 | 22.533 | 32.637 | 48.620 | 1.00 | 27.85 |
| ATOM | 1945 | CA  | TYR | A 25  |        |        |        |      |       |



|      |      |      |     |   |     |        |        |        |      |       |
|------|------|------|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 1959 | O    | VAL | A | 252 | 16.701 | 34.572 | 45.683 | 1.00 | 31.28 |
| ATOM | 1960 | CB   | VAL | A | 252 | 17.477 | 32.314 | 47.337 | 1.00 | 28.37 |
| ATOM | 1961 | CG1  | VAL | A | 252 | 18.252 | 31.009 | 47.541 | 1.00 | 27.04 |
| ATOM | 1962 | CG2  | VAL | A | 252 | 16.639 | 32.723 | 48.572 | 1.00 | 29.19 |
| ATOM | 1963 | N    | TRP | A | 253 | 17.733 | 35.711 | 47.324 | 1.00 | 24.23 |
| ATOM | 1964 | CA   | TRP | A | 253 | 16.883 | 36.868 | 47.152 | 1.00 | 22.27 |
| ATOM | 1965 | C    | TRP | A | 253 | 17.300 | 37.793 | 46.041 | 1.00 | 27.00 |
| ATOM | 1966 | O    | TRP | A | 253 | 16.557 | 38.683 | 45.646 | 1.00 | 27.03 |
| ATOM | 1967 | CB   | TRP | A | 253 | 16.782 | 37.617 | 48.482 | 1.00 | 20.01 |
| ATOM | 1968 | CG   | TRP | A | 253 | 16.465 | 36.613 | 49.516 | 1.00 | 20.82 |
| ATOM | 1969 | CD1  | TRP | A | 253 | 17.322 | 35.799 | 50.186 | 1.00 | 23.01 |
| ATOM | 1970 | CD2  | TRP | A | 253 | 15.137 | 36.270 | 49.921 | 1.00 | 20.48 |
| ATOM | 1971 | NE1  | TRP | A | 253 | 16.601 | 34.977 | 51.043 | 1.00 | 23.74 |
| ATOM | 1972 | CE2  | TRP | A | 253 | 15.254 | 35.266 | 50.904 | 1.00 | 24.56 |
| ATOM | 1973 | CE3  | TRP | A | 253 | 13.882 | 36.771 | 49.588 | 1.00 | 22.14 |
| ATOM | 1974 | CZ2  | TRP | A | 253 | 14.109 | 34.730 | 51.517 | 1.00 | 23.35 |
| ATOM | 1975 | CZ3  | TRP | A | 253 | 12.768 | 36.257 | 50.222 | 1.00 | 23.92 |
| ATOM | 1976 | CH2  | TRP | A | 253 | 12.874 | 35.239 | 51.177 | 1.00 | 23.31 |
| ATOM | 1977 | N    | GLY | A | 254 | 18.501 | 37.611 | 45.545 | 1.00 | 27.81 |
| ATOM | 1978 | CA   | GLY | A | 254 | 18.892 | 38.465 | 44.452 | 1.00 | 28.22 |
| ATOM | 1979 | C    | GLY | A | 254 | 19.621 | 39.697 | 44.909 | 1.00 | 35.44 |
| ATOM | 1980 | O    | GLY | A | 254 | 20.847 | 39.714 | 44.874 | 1.00 | 43.76 |
| ATOM | 1981 | N    | GLN | A | 255 | 18.881 | 40.732 | 45.300 | 1.00 | 27.98 |
| ATOM | 1982 | CA   | GLN | A | 255 | 19.534 | 41.960 | 45.744 | 1.00 | 27.20 |
| ATOM | 1983 | C    | GLN | A | 255 | 19.640 | 42.000 | 47.258 | 1.00 | 29.51 |
| ATOM | 1984 | O    | GLN | A | 255 | 18.806 | 41.408 | 47.954 | 1.00 | 28.12 |
| ATOM | 1985 | CB   | GLN | A | 255 | 18.662 | 43.159 | 45.345 | 1.00 | 28.02 |
| ATOM | 1986 | CG   | GLN | A | 255 | 19.350 | 44.520 | 45.558 | 1.00 | 45.41 |
| ATOM | 1987 | CD   | GLN | A | 255 | 20.484 | 44.770 | 44.589 | 1.00 | 58.13 |
| ATOM | 1988 | OE1  | GLN | A | 255 | 20.911 | 43.848 | 43.877 | 1.00 | 52.27 |
| ATOM | 1989 | NE2  | GLN | A | 255 | 20.982 | 46.004 | 44.575 | 1.00 | 30.88 |
| ATOM | 1990 | N    | TYR | A | 256 | 20.653 | 42.704 | 47.744 | 1.00 | 27.70 |
| ATOM | 1991 | CA   | TYR | A | 256 | 20.809 | 42.901 | 49.172 | 1.00 | 26.42 |
| ATOM | 1992 | C    | TYR | A | 256 | 20.972 | 44.378 | 49.406 | 1.00 | 21.82 |
| ATOM | 1993 | O    | TYR | A | 256 | 22.075 | 44.858 | 49.525 | 1.00 | 23.87 |
| ATOM | 1994 | CB   | TYR | A | 256 | 21.869 | 42.093 | 49.955 | 1.00 | 27.12 |
| ATOM | 1995 | CG   | TYR | A | 256 | 21.726 | 42.369 | 51.460 | 1.00 | 21.81 |
| ATOM | 1996 | CD1  | TYR | A | 256 | 20.740 | 41.730 | 52.215 | 1.00 | 20.63 |
| ATOM | 1997 | CD2  | TYR | A | 256 | 22.547 | 43.282 | 52.130 | 1.00 | 21.46 |
| ATOM | 1998 | CE1  | TYR | A | 256 | 20.573 | 42.001 | 53.579 | 1.00 | 17.95 |
| ATOM | 1999 | CE2  | TYR | A | 256 | 22.405 | 43.573 | 53.490 | 1.00 | 21.50 |
| ATOM | 2000 | CZ   | TYR | A | 256 | 21.412 | 42.913 | 54.223 | 1.00 | 32.29 |
| ATOM | 2001 | OH</ |     |   |     |        |        |        |      |       |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 2017 | CD2 | LEU | A | 258 | 21.538 | 47.060 | 55.152 | 1.00 | 21.84 |
| ATOM | 2018 | N   | LEU | A | 259 | 18.644 | 50.245 | 53.726 | 1.00 | 23.21 |
| ATOM | 2019 | CA  | LEU | A | 259 | 17.936 | 51.484 | 53.915 | 1.00 | 21.37 |
| ATOM | 2020 | C   | LEU | A | 259 | 18.185 | 52.045 | 55.330 | 1.00 | 27.59 |
| ATOM | 2021 | O   | LEU | A | 259 | 17.771 | 51.432 | 56.319 | 1.00 | 26.86 |
| ATOM | 2022 | CB  | LEU | A | 259 | 16.433 | 51.307 | 53.702 | 1.00 | 18.80 |
| ATOM | 2023 | CG  | LEU | A | 259 | 15.667 | 52.543 | 54.132 | 1.00 | 19.47 |
| ATOM | 2024 | CD1 | LEU | A | 259 | 15.857 | 53.670 | 53.128 | 1.00 | 21.23 |
| ATOM | 2025 | CD2 | LEU | A | 259 | 14.192 | 52.205 | 54.204 | 1.00 | 18.79 |
| ATOM | 2026 | N   | VAL | A | 260 | 18.847 | 53.205 | 55.408 | 1.00 | 21.57 |
| ATOM | 2027 | CA  | VAL | A | 260 | 19.111 | 53.903 | 56.648 | 1.00 | 21.30 |
| ATOM | 2028 | C   | VAL | A | 260 | 17.968 | 54.863 | 56.866 | 1.00 | 30.36 |
| ATOM | 2029 | O   | VAL | A | 260 | 17.833 | 55.881 | 56.181 | 1.00 | 31.96 |
| ATOM | 2030 | CB  | VAL | A | 260 | 20.403 | 54.663 | 56.563 | 1.00 | 24.67 |
| ATOM | 2031 | CG1 | VAL | A | 260 | 20.789 | 55.226 | 57.929 | 1.00 | 22.98 |
| ATOM | 2032 | CG2 | VAL | A | 260 | 21.446 | 53.677 | 56.074 | 1.00 | 26.02 |
| ATOM | 2033 | N   | LEU | A | 261 | 17.116 | 54.507 | 57.818 | 1.00 | 23.24 |
| ATOM | 2034 | CA  | LEU | A | 261 | 15.930 | 55.273 | 58.105 | 1.00 | 19.43 |
| ATOM | 2035 | C   | LEU | A | 261 | 16.171 | 56.472 | 58.971 | 1.00 | 23.79 |
| ATOM | 2036 | O   | LEU | A | 261 | 17.278 | 56.708 | 59.443 | 1.00 | 25.06 |
| ATOM | 2037 | CB  | LEU | A | 261 | 14.943 | 54.367 | 58.842 | 1.00 | 19.66 |
| ATOM | 2038 | CG  | LEU | A | 261 | 14.286 | 53.442 | 57.827 | 1.00 | 28.61 |
| ATOM | 2039 | CD1 | LEU | A | 261 | 14.992 | 52.089 | 57.734 | 1.00 | 28.87 |
| ATOM | 2040 | CD2 | LEU | A | 261 | 12.786 | 53.354 | 58.044 | 1.00 | 37.75 |
| ATOM | 2041 | N   | PRO | A | 262 | 15.087 | 57.203 | 59.170 | 1.00 | 25.75 |
| ATOM | 2042 | CA  | PRO | A | 262 | 15.137 | 58.343 | 60.051 | 1.00 | 27.87 |
| ATOM | 2043 | C   | PRO | A | 262 | 15.219 | 57.793 | 61.487 | 1.00 | 29.99 |
| ATOM | 2044 | O   | PRO | A | 262 | 14.875 | 56.636 | 61.792 | 1.00 | 25.40 |
| ATOM | 2045 | CB  | PRO | A | 262 | 13.872 | 59.168 | 59.811 | 1.00 | 28.11 |
| ATOM | 2046 | CG  | PRO | A | 262 | 13.039 | 58.416 | 58.792 | 1.00 | 29.99 |
| ATOM | 2047 | CD  | PRO | A | 262 | 13.722 | 57.078 | 58.569 | 1.00 | 24.33 |
| ATOM | 2048 | N   | PRO | A | 263 | 15.704 | 58.649 | 62.378 | 1.00 | 27.92 |
| ATOM | 2049 | CA  | PRO | A | 263 | 15.950 | 58.306 | 63.776 | 1.00 | 22.66 |
| ATOM | 2050 | C   | PRO | A | 263 | 14.891 | 57.588 | 64.585 | 1.00 | 21.89 |
| ATOM | 2051 | O   | PRO | A | 263 | 15.234 | 56.802 | 65.462 | 1.00 | 22.12 |
| ATOM | 2052 | CB  | PRO | A | 263 | 16.552 | 59.545 | 64.448 | 1.00 | 23.50 |
| ATOM | 2053 | CG  | PRO | A | 263 | 16.866 | 60.527 | 63.325 | 1.00 | 29.26 |
| ATOM | 2054 | CD  | PRO | A | 263 | 16.003 | 60.104 | 62.142 | 1.00 | 26.83 |
| ATOM | 2055 | N   | SER | A | 264 | 13.621 | 57.862 | 64.315 | 1.00 | 21.95 |
| ATOM | 2056 | CA  | SER | A | 264 | 12.531 | 57.219 | 65.037 | 1.00 | 21.99 |
| ATOM | 2057 | C   | SER | A | 264 | 12.344 | 55.765 | 64.610 | 1.00 | 16.88 |
| ATOM | 2058 | O   | SER | A | 264 | 11.457 | 55.099 | 65.134 | 1.00 | 16.95 |
| ATOM | 2059 | CB  | SER | A | 264 | 11.206 | 5      |        |      |       |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 2075 | O   | PRO | A | 266 | 13.354 | 50.045 | 67.733 | 1.00 | 12.99 |
| ATOM | 2076 | CB  | PRO | A | 266 | 10.744 | 50.987 | 66.520 | 1.00 | 15.93 |
| ATOM | 2077 | CG  | PRO | A | 266 | 10.017 | 51.164 | 65.205 | 1.00 | 18.48 |
| ATOM | 2078 | CD  | PRO | A | 266 | 10.879 | 52.008 | 64.308 | 1.00 | 14.04 |
| ATOM | 2079 | N   | TYR | A | 267 | 13.785 | 49.894 | 65.537 | 1.00 | 16.40 |
| ATOM | 2080 | CA  | TYR | A | 267 | 14.752 | 48.813 | 65.694 | 1.00 | 15.75 |
| ATOM | 2081 | C   | TYR | A | 267 | 16.131 | 49.180 | 65.197 | 1.00 | 19.44 |
| ATOM | 2082 | O   | TYR | A | 267 | 16.342 | 50.176 | 64.499 | 1.00 | 18.10 |
| ATOM | 2083 | CB  | TYR | A | 267 | 14.269 | 47.507 | 65.006 | 1.00 | 17.45 |
| ATOM | 2084 | CG  | TYR | A | 267 | 12.954 | 47.043 | 65.626 | 1.00 | 19.30 |
| ATOM | 2085 | CD1 | TYR | A | 267 | 12.992 | 46.238 | 66.766 | 1.00 | 19.19 |
| ATOM | 2086 | CD2 | TYR | A | 267 | 11.705 | 47.435 | 65.127 | 1.00 | 14.85 |
| ATOM | 2087 | CE1 | TYR | A | 267 | 11.806 | 45.817 | 67.369 | 1.00 | 21.05 |
| ATOM | 2088 | CE2 | TYR | A | 267 | 10.512 | 47.032 | 65.734 | 1.00 | 9.78  |
| ATOM | 2089 | CZ  | TYR | A | 267 | 10.563 | 46.208 | 66.861 | 1.00 | 13.87 |
| ATOM | 2090 | OH  | TYR | A | 267 | 9.427  | 45.791 | 67.529 | 1.00 | 15.56 |
| ATOM | 2091 | N   | GLY | A | 268 | 17.091 | 48.353 | 65.583 | 1.00 | 14.17 |
| ATOM | 2092 | CA  | GLY | A | 268 | 18.460 | 48.522 | 65.122 | 1.00 | 15.06 |
| ATOM | 2093 | C   | GLY | A | 268 | 18.508 | 48.085 | 63.652 | 1.00 | 19.31 |
| ATOM | 2094 | O   | GLY | A | 268 | 19.152 | 48.695 | 62.809 | 1.00 | 17.05 |
| ATOM | 2095 | N   | GLY | A | 269 | 17.773 | 47.011 | 63.360 | 1.00 | 18.06 |
| ATOM | 2096 | CA  | GLY | A | 269 | 17.688 | 46.453 | 62.026 | 1.00 | 15.91 |
| ATOM | 2097 | C   | GLY | A | 269 | 16.438 | 45.598 | 61.892 | 1.00 | 16.11 |
| ATOM | 2098 | O   | GLY | A | 269 | 15.869 | 45.183 | 62.891 | 1.00 | 14.41 |
| ATOM | 2099 | N   | MET | A | 270 | 16.031 | 45.376 | 60.637 | 1.00 | 13.94 |
| ATOM | 2100 | CA  | MET | A | 270 | 14.868 | 44.605 | 60.233 | 1.00 | 13.83 |
| ATOM | 2101 | C   | MET | A | 270 | 15.162 | 43.978 | 58.874 | 1.00 | 21.59 |
| ATOM | 2102 | O   | MET | A | 270 | 15.310 | 44.700 | 57.890 | 1.00 | 18.65 |
| ATOM | 2103 | CB  | MET | A | 270 | 13.590 | 45.444 | 60.058 | 1.00 | 16.36 |
| ATOM | 2104 | CG  | MET | A | 270 | 12.450 | 44.562 | 59.571 | 1.00 | 17.70 |
| ATOM | 2105 | SD  | MET | A | 270 | 11.946 | 43.379 | 60.866 | 1.00 | 21.03 |
| ATOM | 2106 | CE  | MET | A | 270 | 11.379 | 41.967 | 59.867 | 1.00 | 19.69 |
| ATOM | 2107 | N   | GLU | A | 271 | 15.249 | 42.647 | 58.859 | 1.00 | 22.89 |
| ATOM | 2108 | CA  | GLU | A | 271 | 15.571 | 41.810 | 57.700 | 1.00 | 18.36 |
| ATOM | 2109 | C   | GLU | A | 271 | 14.546 | 41.835 | 56.562 | 1.00 | 20.73 |
| ATOM | 2110 | O   | GLU | A | 271 | 14.238 | 40.794 | 55.994 | 1.00 | 17.43 |
| ATOM | 2111 | CB  | GLU | A | 271 | 15.852 | 40.352 | 58.174 | 1.00 | 17.49 |
| ATOM | 2112 | CG  | GLU | A | 271 | 14.595 | 39.641 | 58.706 | 1.00 | 14.64 |
| ATOM | 2113 | CD  | GLU | A | 271 | 14.297 | 39.896 | 60.175 | 1.00 | 16.61 |
| ATOM | 2114 | OE1 | GLU | A | 271 | 14.592 | 40.925 | 60.774 | 1.00 | 16.52 |
| ATOM | 2115 | OE2 | GLU | A | 271 | 13.660 | 38.891 | 60.720 | 1.00 | 15.49 |
| ATOM | 2116 | N   | ASN | A | 272 | 13.985 | 42.991 | 56.218 | 1.00 | 16.76 |
| ATOM | 2117 | CA  | ASN | A | 272 | 13     |        |        |      |       |



|      |      |     |           |        |        |        |      |       |
|------|------|-----|-----------|--------|--------|--------|------|-------|
| ATOM | 2133 | C   | CYS A 274 | 16.258 | 44.014 | 49.898 | 1.00 | 27.30 |
| ATOM | 2134 | O   | CYS A 274 | 16.910 | 44.743 | 49.142 | 1.00 | 25.31 |
| ATOM | 2135 | CB  | CYS A 274 | 15.096 | 42.678 | 48.220 | 1.00 | 28.73 |
| ATOM | 2136 | SG  | CYS A 274 | 14.579 | 41.105 | 47.493 | 1.00 | 31.75 |
| ATOM | 2137 | N   | LEU A 275 | 15.729 | 44.378 | 51.073 | 1.00 | 22.65 |
| ATOM | 2138 | CA  | LEU A 275 | 15.850 | 45.744 | 51.607 | 1.00 | 23.25 |
| ATOM | 2139 | C   | LEU A 275 | 15.861 | 45.771 | 53.127 | 1.00 | 24.49 |
| ATOM | 2140 | O   | LEU A 275 | 14.857 | 46.049 | 53.766 | 1.00 | 20.30 |
| ATOM | 2141 | CB  | LEU A 275 | 14.720 | 46.664 | 51.076 | 1.00 | 21.69 |
| ATOM | 2142 | CG  | LEU A 275 | 14.883 | 48.179 | 51.233 | 1.00 | 23.67 |
| ATOM | 2143 | CD1 | LEU A 275 | 16.161 | 48.676 | 50.567 | 1.00 | 21.04 |
| ATOM | 2144 | CD2 | LEU A 275 | 13.678 | 48.860 | 50.598 | 1.00 | 24.01 |
| ATOM | 2145 | N   | THR A 276 | 17.019 | 45.459 | 53.693 | 1.00 | 23.64 |
| ATOM | 2146 | CA  | THR A 276 | 17.168 | 45.522 | 55.142 | 1.00 | 23.40 |
| ATOM | 2147 | C   | THR A 276 | 17.072 | 46.994 | 55.594 | 1.00 | 24.89 |
| ATOM | 2148 | O   | THR A 276 | 17.685 | 47.911 | 55.035 | 1.00 | 21.17 |
| ATOM | 2149 | CB  | THR A 276 | 18.493 | 44.855 | 55.596 | 1.00 | 27.90 |
| ATOM | 2150 | OG1 | THR A 276 | 18.355 | 43.451 | 55.661 | 1.00 | 27.28 |
| ATOM | 2151 | CG2 | THR A 276 | 19.029 | 45.362 | 56.936 | 1.00 | 23.58 |
| ATOM | 2152 | N   | PHE A 277 | 16.247 | 47.234 | 56.612 | 1.00 | 22.02 |
| ATOM | 2153 | CA  | PHE A 277 | 16.088 | 48.573 | 57.195 | 1.00 | 20.16 |
| ATOM | 2154 | C   | PHE A 277 | 17.044 | 48.709 | 58.384 | 1.00 | 25.70 |
| ATOM | 2155 | O   | PHE A 277 | 17.162 | 47.764 | 59.167 | 1.00 | 21.88 |
| ATOM | 2156 | CB  | PHE A 277 | 14.694 | 48.687 | 57.829 | 1.00 | 18.17 |
| ATOM | 2157 | CG  | PHE A 277 | 13.634 | 48.938 | 56.817 | 1.00 | 19.00 |
| ATOM | 2158 | CD1 | PHE A 277 | 13.835 | 48.531 | 55.500 | 1.00 | 24.17 |
| ATOM | 2159 | CD2 | PHE A 277 | 12.427 | 49.542 | 57.152 | 1.00 | 20.88 |
| ATOM | 2160 | CE1 | PHE A 277 | 12.862 | 48.745 | 54.525 | 1.00 | 23.52 |
| ATOM | 2161 | CE2 | PHE A 277 | 11.446 | 49.770 | 56.185 | 1.00 | 26.94 |
| ATOM | 2162 | CZ  | PHE A 277 | 11.659 | 49.364 | 54.865 | 1.00 | 22.89 |
| ATOM | 2163 | N   | VAL A 278 | 17.713 | 49.843 | 58.572 | 1.00 | 20.87 |
| ATOM | 2164 | CA  | VAL A 278 | 18.595 | 49.962 | 59.732 | 1.00 | 19.42 |
| ATOM | 2165 | C   | VAL A 278 | 18.432 | 51.321 | 60.375 | 1.00 | 23.68 |
| ATOM | 2166 | O   | VAL A 278 | 18.086 | 52.292 | 59.711 | 1.00 | 19.82 |
| ATOM | 2167 | CB  | VAL A 278 | 20.094 | 49.721 | 59.491 | 1.00 | 18.82 |
| ATOM | 2168 | CG1 | VAL A 278 | 20.320 | 48.314 | 59.001 | 1.00 | 19.20 |
| ATOM | 2169 | CG2 | VAL A 278 | 20.715 | 50.743 | 58.521 | 1.00 | 15.74 |
| ATOM | 2170 | N   | THR A 279 | 18.751 | 51.374 | 61.655 | 1.00 | 18.56 |
| ATOM | 2171 | CA  | THR A 279 | 18.702 | 52.616 | 62.391 | 1.00 | 18.24 |
| ATOM | 2172 | C   | THR A 279 | 19.889 | 53.506 | 61.996 | 1.00 | 19.64 |
| ATOM | 2173 | O   | THR A 279 | 20.971 | 53.008 | 61.740 | 1.00 | 19.05 |
| ATOM | 2174 | CB  | THR A 279 | 18.821 | 52.343 | 63.921 | 1.00 | 19.60 |
| ATOM | 2175 | OG1 | THR A 279 | 18.895 | 53.595 | 64.581 | 1.00 | 16.90 |
| ATOM | 2176 | CG2 | THR A 279 | 20.120 | 51.588 | 64.205 | 1.00 | 13.57 |
| ATOM | 2177 | N   | PRO A 280 | 19.719 | 54.836 | 61.999 | 1.00 | 19.21 |
| ATOM | 2178 | CA  | PRO A 280 | 20.829 | 55.707 | 61.712 | 1.00 | 18.61 |
| ATOM | 2179 | C   | PRO A 280 | 21.772 | 55.699 | 62.912 | 1.00 | 21.55 |
| ATOM | 2180 | O   | PRO A 280 | 22.918 | 56.168 | 62.799 | 1.00 | 21.21 |
| ATOM | 2181 | CB  | PRO A 280 | 20.267 | 57.113 | 61.511 | 1.00 | 19.88 |
| ATOM | 2182 | CG  | PRO A 280 | 18.901 | 57.068 | 62.176 | 1.00 | 18.63 |
| ATOM | 2183 | CD  | PRO A 280 | 18.448 | 55.624 | 62.007 | 1.00 | 17.87 |
| ATOM | 2184 | N   | THR A 281 | 21.303 | 55.127 | 64.044 | 1.00 | 20.04 |
| ATOM | 2185 | CA  | THR A 281 | 22.174 | 55.031 | 65.214 | 1.00 | 21.24 |
| ATOM | 2186 | C   | THR A 281 | 23.367 | 54.097 | 65.002 | 1.00 | 22.67 |
| ATOM | 2187 | O   | THR A 281 | 24.300 | 54.031 | 65.829 | 1.00 | 20.18 |
| ATOM | 2188 | CB  | THR A 281 | 21.477 | 54.765 | 66.547 | 1.00 | 24.13 |
| ATOM | 2189 | OG1 | THR A 281 | 20.923 | 53.454 | 66.562 | 1.00 | 21.04 |
| ATOM | 2190 | CG2 | THR A 281 | 20.438 | 55.869 | 66.750 | 1.00 | 20.84 |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 2191 | N   | LEU | A | 282 | 23.342 | 53.397 | 63.867 | 1.00 | 16.05 |
| ATOM | 2192 | CA  | LEU | A | 282 | 24.460 | 52.528 | 63.556 | 1.00 | 16.95 |
| ATOM | 2193 | C   | LEU | A | 282 | 25.644 | 53.343 | 63.000 | 1.00 | 23.24 |
| ATOM | 2194 | O   | LEU | A | 282 | 26.768 | 52.846 | 62.861 | 1.00 | 21.40 |
| ATOM | 2195 | CB  | LEU | A | 282 | 24.087 | 51.519 | 62.454 | 1.00 | 16.65 |
| ATOM | 2196 | CG  | LEU | A | 282 | 23.053 | 50.463 | 62.813 | 1.00 | 20.67 |
| ATOM | 2197 | CD1 | LEU | A | 282 | 23.121 | 49.359 | 61.760 | 1.00 | 17.37 |
| ATOM | 2198 | CD2 | LEU | A | 282 | 23.359 | 49.877 | 64.193 | 1.00 | 11.35 |
| ATOM | 2199 | N   | LEU | A | 283 | 25.410 | 54.598 | 62.615 | 1.00 | 19.06 |
| ATOM | 2200 | CA  | LEU | A | 283 | 26.474 | 55.379 | 61.979 | 1.00 | 21.46 |
| ATOM | 2201 | C   | LEU | A | 283 | 27.530 | 55.898 | 62.926 | 1.00 | 29.82 |
| ATOM | 2202 | O   | LEU | A | 283 | 27.608 | 57.107 | 63.129 | 1.00 | 30.36 |
| ATOM | 2203 | CB  | LEU | A | 283 | 25.861 | 56.561 | 61.208 | 1.00 | 20.36 |
| ATOM | 2204 | CG  | LEU | A | 283 | 24.829 | 56.070 | 60.198 | 1.00 | 26.22 |
| ATOM | 2205 | CD1 | LEU | A | 283 | 24.170 | 57.268 | 59.509 | 1.00 | 26.75 |
| ATOM | 2206 | CD2 | LEU | A | 283 | 25.542 | 55.174 | 59.178 | 1.00 | 28.22 |
| ATOM | 2207 | N   | ALA | A | 284 | 28.307 | 54.983 | 63.499 | 1.00 | 24.27 |
| ATOM | 2208 | CA  | ALA | A | 284 | 29.299 | 55.346 | 64.481 | 1.00 | 23.44 |
| ATOM | 2209 | C   | ALA | A | 284 | 30.519 | 55.998 | 63.865 | 1.00 | 30.13 |
| ATOM | 2210 | O   | ALA | A | 284 | 31.280 | 56.659 | 64.566 | 1.00 | 28.42 |
| ATOM | 2211 | CB  | ALA | A | 284 | 29.683 | 54.147 | 65.325 | 1.00 | 23.18 |
| ATOM | 2212 | N   | GLY | A | 285 | 30.706 | 55.829 | 62.561 | 1.00 | 26.03 |
| ATOM | 2213 | CA  | GLY | A | 285 | 31.852 | 56.425 | 61.898 | 1.00 | 23.94 |
| ATOM | 2214 | C   | GLY | A | 285 | 33.106 | 55.548 | 61.857 | 1.00 | 35.38 |
| ATOM | 2215 | O   | GLY | A | 285 | 34.152 | 55.934 | 61.321 | 1.00 | 35.31 |
| ATOM | 2216 | N   | ASP | A | 286 | 33.010 | 54.339 | 62.409 | 1.00 | 29.64 |
| ATOM | 2217 | CA  | ASP | A | 286 | 34.121 | 53.427 | 62.408 | 1.00 | 22.48 |
| ATOM | 2218 | C   | ASP | A | 286 | 33.702 | 52.013 | 62.065 | 1.00 | 22.54 |
| ATOM | 2219 | O   | ASP | A | 286 | 34.484 | 51.120 | 62.321 | 1.00 | 20.43 |
| ATOM | 2220 | CB  | ASP | A | 286 | 34.798 | 53.422 | 63.776 | 1.00 | 22.77 |
| ATOM | 2221 | CG  | ASP | A | 286 | 33.830 | 53.000 | 64.842 | 1.00 | 23.72 |
| ATOM | 2222 | OD1 | ASP | A | 286 | 32.727 | 52.571 | 64.605 | 1.00 | 23.69 |
| ATOM | 2223 | OD2 | ASP | A | 286 | 34.303 | 53.119 | 66.039 | 1.00 | 25.35 |
| ATOM | 2224 | N   | LYS | A | 287 | 32.483 | 51.824 | 61.557 | 1.00 | 18.47 |
| ATOM | 2225 | CA  | LYS | A | 287 | 31.998 | 50.498 | 61.175 | 1.00 | 19.69 |
| ATOM | 2226 | C   | LYS | A | 287 | 31.839 | 49.507 | 62.330 | 1.00 | 23.72 |
| ATOM | 2227 | O   | LYS | A | 287 | 31.524 | 48.328 | 62.143 | 1.00 | 23.33 |
| ATOM | 2228 | CB  | LYS | A | 287 | 32.928 | 49.860 | 60.138 | 1.00 | 23.38 |
| ATOM | 2229 | CG  | LYS | A | 287 | 33.393 | 50.760 | 58.992 | 1.00 | 28.89 |
| ATOM | 2230 | CD  | LYS | A | 287 | 34.194 | 49.994 | 57.933 | 1.00 | 29.02 |
| ATOM | 2231 | CE  | LYS | A | 287 | 35.016 | 50.878 | 56.992 | 1.00 | 29.20 |
| ATOM | 2232 | NZ  | LYS | A | 287 | 34.225 | 51.494 | 55.908 | 1.00 | 31.15 |
| ATOM | 2233 | N   | SER | A | 288 | 32.090 | 49.993 | 63.537 | 1.00 | 23.67 |
| ATOM | 2234 | CA  | SER | A | 288 | 32.033 | 49.195 | 64.756 | 1.00 | 21.48 |
| ATOM | 2235 | C   | SER | A | 288 | 30.681 | 48.520 | 65.080 | 1.00 | 24.82 |
| ATOM | 2236 | O   | SER | A | 288 | 30.644 | 47.530 | 65.833 | 1.00 | 23.30 |
| ATOM | 2237 | CB  | SER | A | 288 | 32.568 | 50.021 | 65.915 | 1.00 | 17.62 |
| ATOM | 2238 | OG  | SER | A | 288 | 31.613 | 50.986 | 66.283 | 1.00 | 22.51 |
| ATOM | 2239 | N   | LEU | A | 289 | 29.577 | 49.068 | 64.546 | 1.00 | 17.98 |
| ATOM | 2240 | CA  | LEU | A | 289 | 28.235 | 48.524 | 64.763 | 1.00 | 17.52 |
| ATOM | 2241 | C   | LEU | A | 289 | 27.719 | 47.621 | 63.632 | 1.00 | 25.16 |
| ATOM | 2242 | O   | LEU | A | 289 | 26.526 | 47.300 | 63.525 | 1.00 | 22.82 |
| ATOM | 2243 | CB  | LEU | A | 289 | 27.236 | 49.616 | 65.156 | 1.00 | 15.28 |
| ATOM | 2244 | CG  | LEU | A | 289 | 27.741 | 50.434 | 66.350 | 1.00 | 20.44 |
| ATOM | 2245 | CD1 | LEU | A | 289 | 26.607 | 51.363 | 66.782 | 1.00 | 18.76 |
| ATOM | 2246 | CD2 | LEU | A | 289 | 28.151 | 49.556 | 67.549 | 1.00 | 14.67 |
| ATOM | 2247 | N   | SER | A | 290 | 28.649 | 47.173 | 62.784 | 1.00 | 20.51 |
| ATOM | 2248 | CA  | SER | A | 290 | 28.298 | 46.332 | 61.655 | 1.00 | 22.41 |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 2249 | C   | SER | A | 290 | 27.734 | 44.950 | 62.011 | 1.00 | 24.28 |
| ATOM | 2250 | O   | SER | A | 290 | 27.186 | 44.251 | 61.157 | 1.00 | 24.24 |
| ATOM | 2251 | CB  | SER | A | 290 | 29.457 | 46.263 | 60.676 | 1.00 | 22.09 |
| ATOM | 2252 | OG  | SER | A | 290 | 30.484 | 45.473 | 61.248 | 1.00 | 25.07 |
| ATOM | 2253 | N   | ASN | A | 291 | 27.873 | 44.530 | 63.261 | 1.00 | 19.37 |
| ATOM | 2254 | CA  | ASN | A | 291 | 27.317 | 43.249 | 63.591 | 1.00 | 18.43 |
| ATOM | 2255 | C   | ASN | A | 291 | 25.826 | 43.236 | 63.256 | 1.00 | 17.33 |
| ATOM | 2256 | O   | ASN | A | 291 | 25.265 | 42.192 | 62.964 | 1.00 | 14.56 |
| ATOM | 2257 | CB  | ASN | A | 291 | 27.513 | 42.937 | 65.085 | 1.00 | 19.46 |
| ATOM | 2258 | CG  | ASN | A | 291 | 26.602 | 43.764 | 65.973 | 1.00 | 20.66 |
| ATOM | 2259 | OD1 | ASN | A | 291 | 26.798 | 44.984 | 66.108 | 1.00 | 17.05 |
| ATOM | 2260 | ND2 | ASN | A | 291 | 25.549 | 43.128 | 66.515 | 1.00 | 16.48 |
| ATOM | 2261 | N   | VAL | A | 292 | 25.177 | 44.399 | 63.318 | 1.00 | 14.47 |
| ATOM | 2262 | CA  | VAL | A | 292 | 23.743 | 44.469 | 63.064 | 1.00 | 13.82 |
| ATOM | 2263 | C   | VAL | A | 292 | 23.510 | 44.099 | 61.629 | 1.00 | 21.19 |
| ATOM | 2264 | O   | VAL | A | 292 | 22.525 | 43.437 | 61.257 | 1.00 | 19.13 |
| ATOM | 2265 | CB  | VAL | A | 292 | 23.176 | 45.855 | 63.358 | 1.00 | 16.20 |
| ATOM | 2266 | CG1 | VAL | A | 292 | 21.717 | 45.989 | 62.910 | 1.00 | 13.99 |
| ATOM | 2267 | CG2 | VAL | A | 292 | 23.375 | 46.193 | 64.832 | 1.00 | 14.21 |
| ATOM | 2268 | N   | ILE | A | 293 | 24.478 | 44.519 | 60.820 | 1.00 | 18.72 |
| ATOM | 2269 | CA  | ILE | A | 293 | 24.388 | 44.196 | 59.388 | 1.00 | 17.35 |
| ATOM | 2270 | C   | ILE | A | 293 | 24.537 | 42.686 | 59.190 | 1.00 | 18.12 |
| ATOM | 2271 | O   | ILE | A | 293 | 23.706 | 42.048 | 58.535 | 1.00 | 20.68 |
| ATOM | 2272 | CB  | ILE | A | 293 | 25.347 | 45.002 | 58.504 | 1.00 | 21.90 |
| ATOM | 2273 | CG1 | ILE | A | 293 | 25.212 | 46.508 | 58.732 | 1.00 | 22.34 |
| ATOM | 2274 | CG2 | ILE | A | 293 | 25.106 | 44.651 | 57.036 | 1.00 | 24.91 |
| ATOM | 2275 | CD1 | ILE | A | 293 | 23.875 | 47.084 | 58.267 | 1.00 | 17.25 |
| ATOM | 2276 | N   | ALA | A | 294 | 25.577 | 42.108 | 59.809 | 1.00 | 14.70 |
| ATOM | 2277 | CA  | ALA | A | 294 | 25.798 | 40.674 | 59.744 | 1.00 | 14.92 |
| ATOM | 2278 | C   | ALA | A | 294 | 24.525 | 39.915 | 60.144 | 1.00 | 19.80 |
| ATOM | 2279 | O   | ALA | A | 294 | 24.134 | 38.879 | 59.613 | 1.00 | 19.51 |
| ATOM | 2280 | CB  | ALA | A | 294 | 26.963 | 40.320 | 60.692 | 1.00 | 11.24 |
| ATOM | 2281 | N   | HIS | A | 295 | 23.858 | 40.467 | 61.141 | 1.00 | 19.87 |
| ATOM | 2282 | CA  | HIS | A | 295 | 22.684 | 39.855 | 61.718 | 1.00 | 17.44 |
| ATOM | 2283 | C   | HIS | A | 295 | 21.564 | 39.788 | 60.725 | 1.00 | 15.33 |
| ATOM | 2284 | O   | HIS | A | 295 | 21.046 | 38.695 | 60.487 | 1.00 | 15.82 |
| ATOM | 2285 | CB  | HIS | A | 295 | 22.243 | 40.560 | 63.038 | 1.00 | 16.85 |
| ATOM | 2286 | CG  | HIS | A | 295 | 20.982 | 40.016 | 63.661 | 1.00 | 14.90 |
| ATOM | 2287 | ND1 | HIS | A | 295 | 21.029 | 39.160 | 64.771 | 1.00 | 13.18 |
| ATOM | 2288 | CD2 | HIS | A | 295 | 19.681 | 40.220 | 63.307 | 1.00 | 14.18 |
| ATOM | 2289 | CE1 | HIS | A | 295 | 19.763 | 38.841 | 65.046 | 1.00 | 12.25 |
| ATOM | 2290 | NE2 | HIS | A | 295 | 18.926 | 39.479 | 64.206 | 1.00 | 13.88 |
| ATOM | 2291 | N   | GLU | A | 296 | 21.201 | 40.970 | 60     |      |       |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 2307 | CD1 | ILE | A | 297 | 25.286 | 41.106 | 55.363 | 1.00 | 18.27 |
| ATOM | 2308 | N   | SER | A | 298 | 22.043 | 37.525 | 57.903 | 1.00 | 19.20 |
| ATOM | 2309 | CA  | SER | A | 298 | 21.828 | 36.138 | 58.327 | 1.00 | 18.22 |
| ATOM | 2310 | C   | SER | A | 298 | 20.386 | 35.663 | 58.269 | 1.00 | 17.45 |
| ATOM | 2311 | O   | SER | A | 298 | 20.138 | 34.479 | 58.073 | 1.00 | 18.23 |
| ATOM | 2312 | CB  | SER | A | 298 | 22.415 | 35.795 | 59.687 | 1.00 | 19.89 |
| ATOM | 2313 | OG  | SER | A | 298 | 23.812 | 35.938 | 59.627 | 1.00 | 20.48 |
| ATOM | 2314 | N   | HIS | A | 299 | 19.458 | 36.589 | 58.479 | 1.00 | 14.42 |
| ATOM | 2315 | CA  | HIS | A | 299 | 18.038 | 36.284 | 58.435 | 1.00 | 14.65 |
| ATOM | 2316 | C   | HIS | A | 299 | 17.620 | 35.833 | 57.031 | 1.00 | 19.88 |
| ATOM | 2317 | O   | HIS | A | 299 | 16.610 | 35.136 | 56.857 | 1.00 | 22.28 |
| ATOM | 2318 | CB  | HIS | A | 299 | 17.235 | 37.515 | 58.891 | 1.00 | 16.87 |
| ATOM | 2319 | CG  | HIS | A | 299 | 16.952 | 37.582 | 60.387 | 1.00 | 18.36 |
| ATOM | 2320 | ND1 | HIS | A | 299 | 16.386 | 36.512 | 61.090 | 1.00 | 15.19 |
| ATOM | 2321 | CD2 | HIS | A | 299 | 17.138 | 38.601 | 61.282 | 1.00 | 14.09 |
| ATOM | 2322 | CE1 | HIS | A | 299 | 16.235 | 36.894 | 62.356 | 1.00 | 13.44 |
| ATOM | 2323 | NE2 | HIS | A | 299 | 16.671 | 38.129 | 62.478 | 1.00 | 13.61 |
| ATOM | 2324 | N   | SER | A | 300 | 18.416 | 36.216 | 56.025 | 1.00 | 16.24 |
| ATOM | 2325 | CA  | SER | A | 300 | 18.121 | 35.813 | 54.635 | 1.00 | 18.63 |
| ATOM | 2326 | C   | SER | A | 300 | 18.061 | 34.297 | 54.485 | 1.00 | 22.35 |
| ATOM | 2327 | O   | SER | A | 300 | 17.696 | 33.798 | 53.426 | 1.00 | 20.36 |
| ATOM | 2328 | CB  | SER | A | 300 | 19.092 | 36.353 | 53.595 | 1.00 | 18.87 |
| ATOM | 2329 | OG  | SER | A | 300 | 19.383 | 37.715 | 53.804 | 1.00 | 19.75 |
| ATOM | 2330 | N   | TRP | A | 301 | 18.469 | 33.616 | 55.557 | 1.00 | 19.18 |
| ATOM | 2331 | CA  | TRP | A | 301 | 18.431 | 32.189 | 55.676 | 1.00 | 21.61 |
| ATOM | 2332 | C   | TRP | A | 301 | 17.572 | 31.826 | 56.889 | 1.00 | 23.56 |
| ATOM | 2333 | O   | TRP | A | 301 | 16.478 | 31.271 | 56.777 | 1.00 | 23.82 |
| ATOM | 2334 | CB  | TRP | A | 301 | 19.815 | 31.539 | 55.793 | 1.00 | 23.04 |
| ATOM | 2335 | CG  | TRP | A | 301 | 20.658 | 31.686 | 54.552 | 1.00 | 25.35 |
| ATOM | 2336 | CD1 | TRP | A | 301 | 20.855 | 30.728 | 53.601 | 1.00 | 27.96 |
| ATOM | 2337 | CD2 | TRP | A | 301 | 21.462 | 32.798 | 54.143 | 1.00 | 23.60 |
| ATOM | 2338 | NE1 | TRP | A | 301 | 21.694 | 31.178 | 52.618 | 1.00 | 23.97 |
| ATOM | 2339 | CE2 | TRP | A | 301 | 22.097 | 32.432 | 52.915 | 1.00 | 23.82 |
| ATOM | 2340 | CE3 | TRP | A | 301 | 21.688 | 34.053 | 54.689 | 1.00 | 22.79 |
| ATOM | 2341 | CZ2 | TRP | A | 301 | 22.939 | 33.272 | 52.216 | 1.00 | 22.46 |
| ATOM | 2342 | CZ3 | TRP | A | 301 | 22.534 | 34.892 | 54.000 | 1.00 | 24.82 |
| ATOM | 2343 | CH2 | TRP | A | 301 | 23.153 | 34.502 | 52.796 | 1.00 | 26.57 |
| ATOM | 2344 | N   | THR | A | 302 | 18.080 | 32.149 | 58.074 | 1.00 | 19.87 |
| ATOM | 2345 | CA  | THR | A | 302 | 17.358 | 31.822 | 59.285 | 1.00 | 20.49 |
| ATOM | 2346 | C   | THR | A | 302 | 16.294 | 32.866 | 59.616 | 1.00 | 20.03 |
| ATOM | 2347 | O   | THR | A | 302 | 16.577 | 33.805 | 60.340 | 1.00 | 20.36 |
| ATOM | 2348 | CB  | THR | A | 302 | 18.309 | 31.537 | 60.479 | 1.00 | 15.81 |
| ATOM | 2349 | OG1 | THR | A | 302 | 19.25  |        |        |      |       |



|      |      |     |     |   |     |        |        |        |      |        |
|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
| ATOM | 2365 | C   | LEU | A | 305 | 13.179 | 29.990 | 55.107 | 1.00 | 24.14  |
| ATOM | 2366 | O   | LEU | A | 305 | 12.183 | 29.414 | 54.657 | 1.00 | 20.26  |
| ATOM | 2367 | CB  | LEU | A | 305 | 15.312 | 30.421 | 53.877 | 1.00 | 20.64  |
| ATOM | 2368 | CG  | LEU | A | 305 | 15.667 | 30.763 | 52.443 | 1.00 | 25.36  |
| ATOM | 2369 | CD1 | LEU | A | 305 | 17.031 | 30.163 | 52.135 | 1.00 | 21.74  |
| ATOM | 2370 | CD2 | LEU | A | 305 | 14.601 | 30.274 | 51.458 | 1.00 | 29.52  |
| ATOM | 2371 | N   | VAL | A | 306 | 13.690 | 29.750 | 56.320 | 1.00 | 22.11  |
| ATOM | 2372 | CA  | VAL | A | 306 | 13.087 | 28.894 | 57.326 | 1.00 | 22.78  |
| ATOM | 2373 | C   | VAL | A | 306 | 12.593 | 29.863 | 58.387 | 1.00 | 20.95  |
| ATOM | 2374 | O   | VAL | A | 306 | 13.360 | 30.606 | 59.023 | 1.00 | 17.13  |
| ATOM | 2375 | CB  | VAL | A | 306 | 13.972 | 27.779 | 57.846 | 1.00 | 26.88  |
| ATOM | 2376 | CG1 | VAL | A | 306 | 15.369 | 28.300 | 58.012 | 1.00 | 30.17  |
| ATOM | 2377 | CG2 | VAL | A | 306 | 13.470 | 27.219 | 59.162 | 1.00 | 24.85  |
| ATOM | 2378 | N   | THR | A | 307 | 11.268 | 29.875 | 58.487 | 1.00 | 19.71  |
| ATOM | 2379 | CA  | THR | A | 307 | 10.533 | 30.800 | 59.346 | 1.00 | 18.22  |
| ATOM | 2380 | C   | THR | A | 307 | 9.839  | 30.176 | 60.539 | 1.00 | 16.26  |
| ATOM | 2381 | O   | THR | A | 307 | 9.262  | 29.105 | 60.437 | 1.00 | 12.74  |
| ATOM | 2382 | CB  | THR | A | 307 | 9.463  | 31.476 | 58.441 | 1.00 | 21.45  |
| ATOM | 2383 | OG1 | THR | A | 307 | 10.078 | 31.965 | 57.280 | 1.00 | 17.92  |
| ATOM | 2384 | CG2 | THR | A | 307 | 8.739  | 32.628 | 59.134 | 1.00 | 11.03  |
| ATOM | 2385 | N   | ASN | A | 308 | 9.840  | 30.870 | 61.679 | 1.00 | 13.09  |
| ATOM | 2386 | CA  | ASN | A | 308 | 9.111  | 30.345 | 62.816 | 1.00 | 14.06  |
| ATOM | 2387 | C   | ASN | A | 308 | 7.633  | 30.248 | 62.421 | 1.00 | 16.30  |
| ATOM | 2388 | O   | ASN | A | 308 | 7.041  | 31.166 | 61.832 | 1.00 | 16.00  |
| ATOM | 2389 | CB  | ASN | A | 308 | 9.277  | 31.223 | 64.092 | 1.00 | 12.92  |
| ATOM | 2390 | CG  | ASN | A | 308 | 9.213  | 32.731 | 63.891 | 1.00 | 20.56  |
| ATOM | 2391 | OD1 | ASN | A | 308 | 9.877  | 33.505 | 64.593 | 1.00 | 19.56  |
| ATOM | 2392 | ND2 | ASN | A | 308 | 8.406  | 33.206 | 62.953 | 1.00 | 16.07  |
| ATOM | 2393 | N   | LYS | A | 309 | 7.004  | 29.141 | 62.729 | 1.00 | 15.40  |
| ATOM | 2394 | CA  | LYS | A | 309 | 5.600  | 28.971 | 62.366 | 1.00 | 15.11  |
| ATOM | 2395 | C   | LYS | A | 309 | 4.607  | 29.891 | 63.122 | 1.00 | 19.89  |
| ATOM | 2396 | O   | LYS | A | 309 | 3.540  | 30.305 | 62.651 | 1.00 | 16.39  |
| ATOM | 2397 | CB  | LYS | A | 309 | 5.279  | 27.493 | 62.491 | 1.00 | 14.57  |
| ATOM | 2398 | CG  | LYS | A | 309 | 3.863  | 27.208 | 62.020 | 1.00 | 19.79  |
| ATOM | 2399 | CD  | LYS | A | 309 | 3.513  | 25.738 | 62.103 | 1.00 | 30.87  |
| ATOM | 2400 | CE  | LYS | A | 309 | 3.169  | 25.135 | 60.754 | 1.00 | 82.87  |
| ATOM | 2401 | NZ  | LYS | A | 309 | 4.126  | 24.100 | 60.326 | 1.00 | 100.00 |
| ATOM | 2402 | N   | THR | A | 310 | 4.930  | 30.182 | 64.367 | 1.00 | 15.49  |
| ATOM | 2403 | CA  | THR | A | 310 | 4.165  | 31.100 | 65.196 | 1.00 | 14.00  |
| ATOM | 2404 | C   | THR | A | 310 | 5.196  | 31.851 | 66.038 | 1.00 | 21.33  |
| ATOM | 2405 | O   | THR | A | 310 | 6.333  | 31.382 | 66.204 | 1.00 | 17.08  |
| ATOM | 2406 | CB  | THR | A | 310 | 3.158  | 30.422 | 66.130 | 1.00 | 23.18  |
| ATOM | 2407 | OG1 | THR | A | 310 | 3.843  | 29.888 | 67.272 | 1.00 | 17.70  |
| ATOM | 2408 | CG2 | THR | A | 310 | 2.354  | 29.366 | 65.357 | 1.00 | 24.41  |
| ATOM | 2409 | N   | TRP | A | 311 | 4.797  | 32.998 | 66.591 | 1.00 | 16.85  |
| ATOM | 2410 | CA  | TRP | A | 311 | 5.703  | 33.779 | 67.408 | 1.00 | 13.14  |
| ATOM | 2411 | C   | TRP | A | 311 | 6.121  | 33.074 | 68.703 | 1.00 | 14.85  |
| ATOM | 2412 | O   | TRP | A | 311 | 7.023  | 33.499 | 69.408 | 1.00 | 16.76  |
| ATOM | 2413 | CB  | TRP | A | 311 | 5.152  | 35.196 | 67.620 | 1.00 | 11.46  |
| ATOM | 2414 | CG  | TRP | A | 311 | 4.878  | 35.825 | 66.301 | 1.00 | 12.77  |
| ATOM | 2415 | CD1 | TRP | A | 311 | 3.661  | 36.134 | 65.773 | 1.00 | 15.35  |
| ATOM | 2416 | CD2 | TRP | A | 311 | 5.867  | 36.192 | 65.320 | 1.00 | 14.76  |
| ATOM | 2417 | NE1 | TRP | A | 311 | 3.809  | 36.710 | 64.528 | 1.00 | 15.45  |
| ATOM | 2418 | CE2 | TRP | A | 311 | 5.167  | 36.734 | 64.217 | 1.00 | 16.76  |
| ATOM | 2419 | CE3 | TRP | A | 311 | 7.265  | 36.090 | 65.283 | 1.00 | 15.71  |
| ATOM | 2420 | CZ2 | TRP | A | 311 | 5.851  | 37.203 | 63.090 | 1.00 | 13.67  |
| ATOM | 2421 | CZ3 | TRP | A | 311 | 7.933  | 36.555 | 64.180 | 1.00 | 16.49  |
| ATOM | 2422 | CH2 | TRP | A | 311 | 7.230  | 37.101 | 63.091 | 1.00 | 17.12  |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 2423 | N   | ASP | A | 312 | 5.490  | 31.969 | 69.043 | 1.00 | 13.30 |
| ATOM | 2424 | CA  | ASP | A | 312 | 5.895  | 31.246 | 70.222 | 1.00 | 16.21 |
| ATOM | 2425 | C   | ASP | A | 312 | 7.274  | 30.591 | 70.003 | 1.00 | 17.53 |
| ATOM | 2426 | O   | ASP | A | 312 | 8.008  | 30.260 | 70.927 | 1.00 | 15.45 |
| ATOM | 2427 | CB  | ASP | A | 312 | 4.866  | 30.143 | 70.538 | 1.00 | 17.39 |
| ATOM | 2428 | CG  | ASP | A | 312 | 3.597  | 30.710 | 71.126 | 1.00 | 16.83 |
| ATOM | 2429 | OD1 | ASP | A | 312 | 3.467  | 31.852 | 71.479 | 1.00 | 19.29 |
| ATOM | 2430 | OD2 | ASP | A | 312 | 2.658  | 29.837 | 71.234 | 1.00 | 22.09 |
| ATOM | 2431 | N   | HIS | A | 313 | 7.628  | 30.392 | 68.748 | 1.00 | 13.40 |
| ATOM | 2432 | CA  | HIS | A | 313 | 8.881  | 29.767 | 68.392 | 1.00 | 11.86 |
| ATOM | 2433 | C   | HIS | A | 313 | 9.855  | 30.779 | 67.820 | 1.00 | 14.51 |
| ATOM | 2434 | O   | HIS | A | 313 | 10.768 | 30.463 | 67.080 | 1.00 | 17.00 |
| ATOM | 2435 | CB  | HIS | A | 313 | 8.547  | 28.724 | 67.308 | 1.00 | 14.08 |
| ATOM | 2436 | CG  | HIS | A | 313 | 7.649  | 27.679 | 67.892 | 1.00 | 16.09 |
| ATOM | 2437 | ND1 | HIS | A | 313 | 8.144  | 26.653 | 68.689 | 1.00 | 15.85 |
| ATOM | 2438 | CD2 | HIS | A | 313 | 6.287  | 27.557 | 67.842 | 1.00 | 13.64 |
| ATOM | 2439 | CE1 | HIS | A | 313 | 7.097  | 25.922 | 69.096 | 1.00 | 14.23 |
| ATOM | 2440 | NE2 | HIS | A | 313 | 5.985  | 26.458 | 68.615 | 1.00 | 13.52 |
| ATOM | 2441 | N   | PHE | A | 314 | 9.654  | 32.022 | 68.178 | 1.00 | 14.17 |
| ATOM | 2442 | CA  | PHE | A | 314 | 10.435 | 33.140 | 67.723 | 1.00 | 13.18 |
| ATOM | 2443 | C   | PHE | A | 314 | 11.910 | 32.890 | 67.944 | 1.00 | 13.98 |
| ATOM | 2444 | O   | PHE | A | 314 | 12.775 | 33.355 | 67.210 | 1.00 | 13.88 |
| ATOM | 2445 | CB  | PHE | A | 314 | 9.968  | 34.367 | 68.516 | 1.00 | 11.94 |
| ATOM | 2446 | CG  | PHE | A | 314 | 10.644 | 35.668 | 68.130 | 1.00 | 16.32 |
| ATOM | 2447 | CD1 | PHE | A | 314 | 10.734 | 36.090 | 66.802 | 1.00 | 15.58 |
| ATOM | 2448 | CD2 | PHE | A | 314 | 11.163 | 36.510 | 69.121 | 1.00 | 16.22 |
| ATOM | 2449 | CE1 | PHE | A | 314 | 11.326 | 37.314 | 66.482 | 1.00 | 15.39 |
| ATOM | 2450 | CE2 | PHE | A | 314 | 11.779 | 37.727 | 68.826 | 1.00 | 17.56 |
| ATOM | 2451 | CZ  | PHE | A | 314 | 11.857 | 38.128 | 67.490 | 1.00 | 16.63 |
| ATOM | 2452 | N   | TRP | A | 315 | 12.244 | 32.131 | 68.950 | 1.00 | 11.22 |
| ATOM | 2453 | CA  | TRP | A | 315 | 13.701 | 31.921 | 69.150 | 1.00 | 8.85  |
| ATOM | 2454 | C   | TRP | A | 315 | 14.386 | 31.236 | 67.968 | 1.00 | 16.46 |
| ATOM | 2455 | O   | TRP | A | 315 | 15.577 | 31.416 | 67.735 | 1.00 | 17.37 |
| ATOM | 2456 | CB  | TRP | A | 315 | 13.968 | 31.130 | 70.425 | 1.00 | 7.05  |
| ATOM | 2457 | CG  | TRP | A | 315 | 13.737 | 29.668 | 70.223 | 1.00 | 11.50 |
| ATOM | 2458 | CD1 | TRP | A | 315 | 12.552 | 28.982 | 70.289 | 1.00 | 14.09 |
| ATOM | 2459 | CD2 | TRP | A | 315 | 14.755 | 28.696 | 69.909 | 1.00 | 14.05 |
| ATOM | 2460 | NE1 | TRP | A | 315 | 12.757 | 27.639 | 70.053 | 1.00 | 14.75 |
| ATOM | 2461 | CE2 | TRP | A | 315 | 14.112 | 27.426 | 69.829 | 1.00 | 19.21 |
| ATOM | 2462 | CE3 | TRP | A | 315 | 16.135 | 28.783 | 69.668 | 1.00 | 14.13 |
| ATOM | 2463 | CZ2 | TRP | A | 315 | 14.854 | 26.239 | 69.553 | 1.00 | 18.59 |
| ATOM | 2464 | CZ3 | TRP | A | 315 | 16.848 | 27.603 | 69.408 | 1.00 | 15.80 |
| ATOM | 2465 | CH2 | TRP | A | 315 | 16.225 | 26.341 |        |      |       |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 2481 | ND2 | ASN | A | 317 | 11.761 | 34.856 | 62.180 | 1.00 | 15.57 |
| ATOM | 2482 | N   | GLU | A | 318 | 15.486 | 34.281 | 65.789 | 1.00 | 15.19 |
| ATOM | 2483 | CA  | GLU | A | 318 | 16.522 | 35.073 | 66.433 | 1.00 | 11.97 |
| ATOM | 2484 | C   | GLU | A | 318 | 17.754 | 34.318 | 66.948 | 1.00 | 14.90 |
| ATOM | 2485 | O   | GLU | A | 318 | 18.861 | 34.762 | 66.724 | 1.00 | 14.03 |
| ATOM | 2486 | CB  | GLU | A | 318 | 15.894 | 36.023 | 67.500 | 1.00 | 9.48  |
| ATOM | 2487 | CG  | GLU | A | 318 | 14.862 | 36.983 | 66.862 | 1.00 | 8.24  |
| ATOM | 2488 | CD  | GLU | A | 318 | 15.409 | 37.898 | 65.776 | 1.00 | 14.75 |
| ATOM | 2489 | OE1 | GLU | A | 318 | 16.597 | 38.104 | 65.536 | 1.00 | 13.03 |
| ATOM | 2490 | OE2 | GLU | A | 318 | 14.468 | 38.428 | 65.046 | 1.00 | 13.56 |
| ATOM | 2491 | N   | GLY | A | 319 | 17.586 | 33.196 | 67.672 | 1.00 | 11.86 |
| ATOM | 2492 | CA  | GLY | A | 319 | 18.740 | 32.468 | 68.173 | 1.00 | 11.63 |
| ATOM | 2493 | C   | GLY | A | 319 | 19.655 | 31.995 | 67.047 | 1.00 | 16.47 |
| ATOM | 2494 | O   | GLY | A | 319 | 20.862 | 32.192 | 67.142 | 1.00 | 16.49 |
| ATOM | 2495 | N   | HIS | A | 320 | 19.118 | 31.374 | 65.991 | 1.00 | 13.41 |
| ATOM | 2496 | CA  | HIS | A | 320 | 19.963 | 30.915 | 64.885 | 1.00 | 13.77 |
| ATOM | 2497 | C   | HIS | A | 320 | 20.671 | 32.086 | 64.195 | 1.00 | 14.09 |
| ATOM | 2498 | O   | HIS | A | 320 | 21.808 | 32.000 | 63.739 | 1.00 | 17.34 |
| ATOM | 2499 | CB  | HIS | A | 320 | 19.148 | 30.128 | 63.832 | 1.00 | 12.48 |
| ATOM | 2500 | CG  | HIS | A | 320 | 18.795 | 28.772 | 64.335 | 1.00 | 16.54 |
| ATOM | 2501 | ND1 | HIS | A | 320 | 17.663 | 28.555 | 65.111 | 1.00 | 18.54 |
| ATOM | 2502 | CD2 | HIS | A | 320 | 19.459 | 27.585 | 64.203 | 1.00 | 19.71 |
| ATOM | 2503 | CE1 | HIS | A | 320 | 17.644 | 27.262 | 65.413 | 1.00 | 17.18 |
| ATOM | 2504 | NE2 | HIS | A | 320 | 18.699 | 26.647 | 64.875 | 1.00 | 17.83 |
| ATOM | 2505 | N   | THR | A | 321 | 19.952 | 33.190 | 64.090 | 1.00 | 12.05 |
| ATOM | 2506 | CA  | THR | A | 321 | 20.492 | 34.376 | 63.465 | 1.00 | 15.46 |
| ATOM | 2507 | C   | THR | A | 321 | 21.669 | 34.999 | 64.244 | 1.00 | 20.32 |
| ATOM | 2508 | O   | THR | A | 321 | 22.678 | 35.421 | 63.665 | 1.00 | 17.11 |
| ATOM | 2509 | CB  | THR | A | 321 | 19.406 | 35.394 | 63.078 | 1.00 | 19.10 |
| ATOM | 2510 | OG1 | THR | A | 321 | 18.517 | 34.726 | 62.203 | 1.00 | 14.48 |
| ATOM | 2511 | CG2 | THR | A | 321 | 20.089 | 36.593 | 62.382 | 1.00 | 12.29 |
| ATOM | 2512 | N   | VAL | A | 322 | 21.541 | 35.047 | 65.573 | 1.00 | 13.35 |
| ATOM | 2513 | CA  | VAL | A | 322 | 22.615 | 35.545 | 66.391 | 1.00 | 12.65 |
| ATOM | 2514 | C   | VAL | A | 322 | 23.795 | 34.588 | 66.234 | 1.00 | 16.03 |
| ATOM | 2515 | O   | VAL | A | 322 | 24.959 | 34.956 | 66.195 | 1.00 | 16.36 |
| ATOM | 2516 | CB  | VAL | A | 322 | 22.149 | 35.593 | 67.838 | 1.00 | 12.95 |
| ATOM | 2517 | CG1 | VAL | A | 322 | 23.340 | 35.917 | 68.744 | 1.00 | 12.06 |
| ATOM | 2518 | CG2 | VAL | A | 322 | 21.070 | 36.690 | 67.972 | 1.00 | 11.64 |
| ATOM | 2519 | N   | TYR | A | 323 | 23.484 | 33.319 | 66.107 | 1.00 | 12.22 |
| ATOM | 2520 | CA  | TYR | A | 323 | 24.543 | 32.350 | 65.974 | 1.00 | 10.51 |
| ATOM | 2521 | C   | TYR | A | 323 | 25.297 | 32.597 | 64.670 | 1.00 | 15.55 |
| ATOM | 2522 | O   | TYR | A | 323 | 26.534 | 32.680 | 64.604 | 1.00 | 15.83 |
| ATOM | 2523 | CB  | TYR | A | 323 | 23.955 |        |        |      |       |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 2539 | N   | GLU | A | 325 | 25.332 | 35.361 | 62.859 | 1.00 | 15.47 |
| ATOM | 2540 | CA  | GLU | A | 325 | 25.885 | 36.694 | 63.007 | 1.00 | 13.65 |
| ATOM | 2541 | C   | GLU | A | 325 | 27.246 | 36.636 | 63.628 | 1.00 | 16.34 |
| ATOM | 2542 | O   | GLU | A | 325 | 28.168 | 37.246 | 63.123 | 1.00 | 15.36 |
| ATOM | 2543 | CB  | GLU | A | 325 | 24.988 | 37.464 | 63.996 | 1.00 | 16.31 |
| ATOM | 2544 | CG  | GLU | A | 325 | 25.472 | 38.890 | 64.363 | 1.00 | 20.54 |
| ATOM | 2545 | CD  | GLU | A | 325 | 24.743 | 39.395 | 65.599 | 1.00 | 30.10 |
| ATOM | 2546 | OE1 | GLU | A | 325 | 23.641 | 39.008 | 65.966 | 1.00 | 18.40 |
| ATOM | 2547 | OE2 | GLU | A | 325 | 25.421 | 40.260 | 66.301 | 1.00 | 21.65 |
| ATOM | 2548 | N   | ARG | A | 326 | 27.329 | 35.892 | 64.727 | 1.00 | 15.29 |
| ATOM | 2549 | CA  | ARG | A | 326 | 28.565 | 35.781 | 65.469 | 1.00 | 14.94 |
| ATOM | 2550 | C   | ARG | A | 326 | 29.651 | 35.048 | 64.718 | 1.00 | 18.22 |
| ATOM | 2551 | O   | ARG | A | 326 | 30.828 | 35.316 | 64.914 | 1.00 | 16.55 |
| ATOM | 2552 | CB  | ARG | A | 326 | 28.367 | 35.352 | 66.915 | 1.00 | 15.15 |
| ATOM | 2553 | CG  | ARG | A | 326 | 27.548 | 36.410 | 67.619 | 1.00 | 11.35 |
| ATOM | 2554 | CD  | ARG | A | 326 | 27.266 | 36.102 | 69.095 | 1.00 | 11.37 |
| ATOM | 2555 | NE  | ARG | A | 326 | 26.619 | 37.266 | 69.724 | 1.00 | 14.76 |
| ATOM | 2556 | CZ  | ARG | A | 326 | 25.805 | 37.229 | 70.769 | 1.00 | 16.13 |
| ATOM | 2557 | NH1 | ARG | A | 326 | 25.523 | 36.107 | 71.419 | 1.00 | 8.40  |
| ATOM | 2558 | NH2 | ARG | A | 326 | 25.262 | 38.379 | 71.166 | 1.00 | 16.43 |
| ATOM | 2559 | N   | HIS | A | 327 | 29.233 | 34.146 | 63.843 | 1.00 | 17.38 |
| ATOM | 2560 | CA  | HIS | A | 327 | 30.174 | 33.400 | 63.018 | 1.00 | 19.62 |
| ATOM | 2561 | C   | HIS | A | 327 | 30.700 | 34.341 | 61.938 | 1.00 | 18.88 |
| ATOM | 2562 | O   | HIS | A | 327 | 31.866 | 34.359 | 61.573 | 1.00 | 19.41 |
| ATOM | 2563 | CB  | HIS | A | 327 | 29.485 | 32.146 | 62.407 | 1.00 | 17.97 |
| ATOM | 2564 | CG  | HIS | A | 327 | 29.698 | 30.875 | 63.188 | 1.00 | 19.10 |
| ATOM | 2565 | ND1 | HIS | A | 327 | 30.973 | 30.414 | 63.524 | 1.00 | 20.08 |
| ATOM | 2566 | CD2 | HIS | A | 327 | 28.792 | 29.954 | 63.642 | 1.00 | 18.16 |
| ATOM | 2567 | CE1 | HIS | A | 327 | 30.824 | 29.266 | 64.188 | 1.00 | 18.80 |
| ATOM | 2568 | NE2 | HIS | A | 327 | 29.519 | 28.976 | 64.284 | 1.00 | 19.69 |
| ATOM | 2569 | N   | ILE | A | 328 | 29.827 | 35.168 | 61.391 | 1.00 | 14.60 |
| ATOM | 2570 | CA  | ILE | A | 328 | 30.304 | 36.097 | 60.362 | 1.00 | 15.76 |
| ATOM | 2571 | C   | ILE | A | 328 | 31.423 | 36.971 | 60.935 | 1.00 | 28.02 |
| ATOM | 2572 | O   | ILE | A | 328 | 32.504 | 37.099 | 60.355 | 1.00 | 26.14 |
| ATOM | 2573 | CB  | ILE | A | 328 | 29.145 | 36.946 | 59.788 | 1.00 | 16.17 |
| ATOM | 2574 | CG1 | ILE | A | 328 | 28.220 | 36.087 | 58.911 | 1.00 | 19.03 |
| ATOM | 2575 | CG2 | ILE | A | 328 | 29.642 | 38.126 | 58.968 | 1.00 | 18.66 |
| ATOM | 2576 | CD1 | ILE | A | 328 | 26.852 | 36.718 | 58.595 | 1.00 | 14.57 |
| ATOM | 2577 | N   | CYS | A | 329 | 31.139 | 37.562 | 62.116 | 1.00 | 21.94 |
| ATOM | 2578 | CA  | CYS | A | 329 | 32.040 | 38.433 | 62.826 | 1.00 | 19.84 |
| ATOM | 2579 | C   | CYS | A | 329 | 33.306 | 37.718 | 63.233 | 1.00 | 20.23 |
| ATOM | 2580 | O   | CYS | A | 329 | 34.391 | 38.278 | 63.154 | 1.00 | 21.18 |
| ATOM | 2581 | CB  | CYS | A | 329 | 31.309 | 39.092 | 64.007 | 1.00 | 26.30 |
| ATOM | 2582 | SG  | CYS | A | 329 | 30.024 | 40.241 | 63.391 | 1.00 | 33.21 |
| ATOM | 2583 | N   | GLY | A | 330 | 33.169 | 36.480 | 63.655 | 1.00 | 17.16 |
| ATOM | 2584 | CA  | GLY | A | 330 | 34.314 | 35.683 | 64.039 | 1.00 | 17.88 |
| ATOM | 2585 | C   | GLY | A | 330 | 35.160 | 35.471 | 62.786 | 1.00 | 23.13 |
| ATOM | 2586 | O   | GLY | A | 330 | 36.381 | 35.479 | 62.773 | 1.00 | 19.20 |
| ATOM | 2587 | N   | ARG | A | 331 | 34.494 | 35.297 | 61.673 | 1.00 | 23.41 |
| ATOM | 2588 | CA  | ARG | A | 331 | 35.238 | 35.107 | 60.454 | 1.00 | 25.42 |
| ATOM | 2589 | C   | ARG | A | 331 | 35.949 | 36.374 | 60.013 | 1.00 | 27.08 |
| ATOM | 2590 | O   | ARG | A | 331 | 37.066 | 36.354 | 59.519 | 1.00 | 30.59 |
| ATOM | 2591 | CB  | ARG | A | 331 | 34.323 | 34.671 | 59.328 | 1.00 | 29.56 |
| ATOM | 2592 | CG  | ARG | A | 331 | 34.103 | 33.178 | 59.357 | 1.00 | 42.38 |
| ATOM | 2593 | CD  | ARG | A | 331 | 34.542 | 32.499 | 58.075 | 1.00 | 45.62 |
| ATOM | 2594 | NE  | ARG | A | 331 | 33.755 | 31.307 | 57.851 | 1.00 | 59.13 |
| ATOM | 2595 | CZ  | ARG | A | 331 | 33.469 | 30.431 | 58.821 | 1.00 | 84.69 |
| ATOM | 2596 | NH1 | ARG | A | 331 | 33.882 | 30.552 | 60.089 | 1.00 | 53.45 |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 2597 | NH2 | ARG | A | 331 | 32.744 | 29.367 | 58.501 | 1.00 | 89.38 |
| ATOM | 2598 | N   | LEU | A | 332 | 35.309 | 37.506 | 60.144 | 1.00 | 18.29 |
| ATOM | 2599 | CA  | LEU | A | 332 | 35.960 | 38.699 | 59.689 | 1.00 | 18.18 |
| ATOM | 2600 | C   | LEU | A | 332 | 36.972 | 39.217 | 60.683 | 1.00 | 27.48 |
| ATOM | 2601 | O   | LEU | A | 332 | 37.943 | 39.809 | 60.248 | 1.00 | 26.78 |
| ATOM | 2602 | CB  | LEU | A | 332 | 34.892 | 39.790 | 59.583 | 1.00 | 20.70 |
| ATOM | 2603 | CG  | LEU | A | 332 | 34.604 | 40.445 | 58.237 | 1.00 | 29.09 |
| ATOM | 2604 | CD1 | LEU | A | 332 | 34.898 | 39.569 | 57.036 | 1.00 | 26.07 |
| ATOM | 2605 | CD2 | LEU | A | 332 | 33.138 | 40.831 | 58.200 | 1.00 | 29.25 |
| ATOM | 2606 | N   | PHE | A | 333 | 36.721 | 39.049 | 61.995 | 1.00 | 21.64 |
| ATOM | 2607 | CA  | PHE | A | 333 | 37.570 | 39.583 | 63.050 | 1.00 | 20.45 |
| ATOM | 2608 | C   | PHE | A | 333 | 38.248 | 38.620 | 63.966 | 1.00 | 21.67 |
| ATOM | 2609 | O   | PHE | A | 333 | 39.050 | 39.031 | 64.794 | 1.00 | 27.38 |
| ATOM | 2610 | CB  | PHE | A | 333 | 36.882 | 40.672 | 63.907 | 1.00 | 23.81 |
| ATOM | 2611 | CG  | PHE | A | 333 | 36.150 | 41.625 | 62.994 | 1.00 | 25.90 |
| ATOM | 2612 | CD1 | PHE | A | 333 | 36.871 | 42.470 | 62.151 | 1.00 | 27.97 |
| ATOM | 2613 | CD2 | PHE | A | 333 | 34.757 | 41.624 | 62.931 | 1.00 | 27.62 |
| ATOM | 2614 | CE1 | PHE | A | 333 | 36.198 | 43.314 | 61.269 | 1.00 | 30.62 |
| ATOM | 2615 | CE2 | PHE | A | 333 | 34.069 | 42.462 | 62.053 | 1.00 | 32.30 |
| ATOM | 2616 | CZ  | PHE | A | 333 | 34.804 | 43.309 | 61.221 | 1.00 | 30.11 |
| ATOM | 2617 | N   | GLY | A | 334 | 37.950 | 37.362 | 63.877 | 1.00 | 17.26 |
| ATOM | 2618 | CA  | GLY | A | 334 | 38.653 | 36.481 | 64.791 | 1.00 | 18.41 |
| ATOM | 2619 | C   | GLY | A | 334 | 37.735 | 35.732 | 65.735 | 1.00 | 23.30 |
| ATOM | 2620 | O   | GLY | A | 334 | 36.758 | 36.276 | 66.244 | 1.00 | 21.87 |
| ATOM | 2621 | N   | GLU | A | 335 | 38.100 | 34.471 | 65.947 | 1.00 | 18.34 |
| ATOM | 2622 | CA  | GLU | A | 335 | 37.377 | 33.558 | 66.821 | 1.00 | 20.82 |
| ATOM | 2623 | C   | GLU | A | 335 | 37.301 | 34.102 | 68.238 | 1.00 | 20.81 |
| ATOM | 2624 | O   | GLU | A | 335 | 36.341 | 33.888 | 68.975 | 1.00 | 20.60 |
| ATOM | 2625 | CB  | GLU | A | 335 | 38.057 | 32.183 | 66.811 | 1.00 | 19.30 |
| ATOM | 2626 | CG  | GLU | A | 335 | 37.366 | 31.179 | 67.751 | 1.00 | 22.22 |
| ATOM | 2627 | CD  | GLU | A | 335 | 35.963 | 30.786 | 67.350 | 1.00 | 22.99 |
| ATOM | 2628 | OE1 | GLU | A | 335 | 35.278 | 31.338 | 66.513 | 1.00 | 26.34 |
| ATOM | 2629 | OE2 | GLU | A | 335 | 35.554 | 29.762 | 68.020 | 1.00 | 20.74 |
| ATOM | 2630 | N   | LYS | A | 336 | 38.327 | 34.845 | 68.615 | 1.00 | 17.24 |
| ATOM | 2631 | CA  | LYS | A | 336 | 38.375 | 35.413 | 69.947 | 1.00 | 16.83 |
| ATOM | 2632 | C   | LYS | A | 336 | 37.316 | 36.470 | 70.050 | 1.00 | 17.51 |
| ATOM | 2633 | O   | LYS | A | 336 | 36.732 | 36.668 | 71.110 | 1.00 | 17.26 |
| ATOM | 2634 | CB  | LYS | A | 336 | 39.735 | 36.002 | 70.264 | 1.00 | 16.58 |
| ATOM | 2635 | CG  | LYS | A | 336 | 40.725 | 34.912 | 70.659 | 1.00 | 20.77 |
| ATOM | 2636 | CD  | LYS | A | 336 | 42.162 | 35.378 | 70.871 | 1.00 | 32.80 |
| ATOM | 2637 | CE  | LYS | A | 336 | 43.184 | 34.329 | 70.432 | 1.00 | 66.91 |
| ATOM | 2638 | NZ  | LYS | A | 336 | 44.484 | 34.418 | 71.112 | 1.00 | 80.02 |
| ATOM | 2639 | N   | PHE | A | 337 | 37.094 | 37.146 | 68.927 | 1.00 | 11.07 |
| ATOM | 2640 | CA  | PHE | A | 337 | 36.075 | 38.183 | 68.893 | 1.00 | 13.51 |
| ATOM | 2641 | C   | PHE | A | 337 | 34.691 | 37.519 | 68.993 | 1.00 | 18.73 |
| ATOM | 2642 | O   | PHE | A | 337 | 33.797 | 37.992 | 69.659 | 1.00 | 15.94 |
| ATOM | 2643 | CB  | PHE | A | 337 | 36.113 | 38.963 | 67.569 | 1.00 | 14.14 |
| ATOM | 2644 | CG  | PHE | A | 337 | 35.241 | 40.194 | 67.632 | 1.00 | 19.04 |
| ATOM | 2645 | CD1 | PHE | A | 337 | 35.266 | 41.054 | 68.734 | 1.00 | 23.19 |
| ATOM | 2646 | CD2 | PHE | A | 337 | 34.406 | 40.562 | 66.571 | 1.00 | 25.81 |
| ATOM | 2647 | CE1 | PHE | A | 337 | 34.473 | 42.209 | 68.789 | 1.00 | 26.28 |
| ATOM | 2648 | CE2 | PHE | A | 337 | 33.634 | 41.727 | 66.594 | 1.00 | 26.38 |
| ATOM | 2649 | CZ  | PHE | A | 337 | 33.645 | 42.557 | 67.718 | 1.00 | 25.06 |
| ATOM | 2650 | N   | ARG | A | 338 | 34.501 | 36.384 | 68.327 | 1.00 | 16.12 |
| ATOM | 2651 | CA  | ARG | A | 338 | 33.239 | 35.665 | 68.384 | 1.00 | 15.03 |
| ATOM | 2652 | C   | ARG | A | 338 | 32.936 | 35.314 | 69.804 | 1.00 | 18.17 |
| ATOM | 2653 | O   | ARG | A | 338 | 31.806 | 35.480 | 70.240 | 1.00 | 18.12 |
| ATOM | 2654 | CB  | ARG | A | 338 | 33.294 | 34.359 | 67.617 | 1.00 | 11.66 |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 2655 | CG  | ARG | A | 338 | 31.961 | 33.629 | 67.660 | 1.00 | 12.35 |
| ATOM | 2656 | CD  | ARG | A | 338 | 31.899 | 32.552 | 66.583 | 1.00 | 17.19 |
| ATOM | 2657 | NE  | ARG | A | 338 | 32.554 | 31.328 | 67.051 | 1.00 | 17.53 |
| ATOM | 2658 | CZ  | ARG | A | 338 | 31.981 | 30.175 | 67.417 | 1.00 | 23.05 |
| ATOM | 2659 | NH1 | ARG | A | 338 | 30.670 | 29.953 | 67.424 | 1.00 | 16.55 |
| ATOM | 2660 | NH2 | ARG | A | 338 | 32.772 | 29.179 | 67.803 | 1.00 | 12.25 |
| ATOM | 2661 | N   | HIS | A | 339 | 33.956 | 34.816 | 70.504 | 1.00 | 12.76 |
| ATOM | 2662 | CA  | HIS | A | 339 | 33.772 | 34.426 | 71.888 | 1.00 | 13.75 |
| ATOM | 2663 | C   | HIS | A | 339 | 33.408 | 35.617 | 72.756 | 1.00 | 18.91 |
| ATOM | 2664 | O   | HIS | A | 339 | 32.587 | 35.520 | 73.655 | 1.00 | 12.72 |
| ATOM | 2665 | CB  | HIS | A | 339 | 35.006 | 33.697 | 72.480 | 1.00 | 14.46 |
| ATOM | 2666 | CG  | HIS | A | 339 | 34.975 | 32.250 | 72.096 | 1.00 | 14.96 |
| ATOM | 2667 | ND1 | HIS | A | 339 | 34.952 | 31.249 | 73.046 | 1.00 | 15.14 |
| ATOM | 2668 | CD2 | HIS | A | 339 | 34.943 | 31.693 | 70.855 | 1.00 | 15.02 |
| ATOM | 2669 | CE1 | HIS | A | 339 | 34.914 | 30.101 | 72.405 | 1.00 | 12.56 |
| ATOM | 2670 | NE2 | HIS | A | 339 | 34.895 | 30.343 | 71.097 | 1.00 | 15.39 |
| ATOM | 2671 | N   | PHE | A | 340 | 34.066 | 36.739 | 72.487 | 1.00 | 16.25 |
| ATOM | 2672 | CA  | PHE | A | 340 | 33.832 | 37.961 | 73.250 | 1.00 | 13.96 |
| ATOM | 2673 | C   | PHE | A | 340 | 32.361 | 38.397 | 73.164 | 1.00 | 16.27 |
| ATOM | 2674 | O   | PHE | A | 340 | 31.700 | 38.760 | 74.158 | 1.00 | 13.82 |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 2675 | CB  | PHE | A | 340 | 34.823 | 39.032 | 72.753 | 1.00 | 11.82 |
| ATOM | 2676 | CG  | PHE | A | 340 | 34.525 | 40.414 | 73.286 | 1.00 | 14.06 |
| ATOM | 2677 | CD1 | PHE | A | 340 | 35.064 | 40.835 | 74.503 | 1.00 | 13.72 |
| ATOM | 2678 | CD2 | PHE | A | 340 | 33.703 | 41.284 | 72.566 | 1.00 | 16.13 |
| ATOM | 2679 | CE1 | PHE | A | 340 | 34.753 | 42.091 | 75.016 | 1.00 | 8.85  |
| ATOM | 2680 | CE2 | PHE | A | 340 | 33.401 | 42.560 | 73.044 | 1.00 | 16.77 |
| ATOM | 2681 | CZ  | PHE | A | 340 | 33.937 | 42.946 | 74.273 | 1.00 | 11.27 |
| ATOM | 2682 | N   | ASN | A | 341 | 31.871 | 38.363 | 71.925 | 1.00 | 13.64 |
| ATOM | 2683 | CA  | ASN | A | 341 | 30.507 | 38.730 | 71.637 | 1.00 | 15.75 |
| ATOM | 2684 | C   | ASN | A | 341 | 29.529 | 37.762 | 72.257 | 1.00 | 18.72 |
| ATOM | 2685 | O   | ASN | A | 341 | 28.446 | 38.129 | 72.717 | 1.00 | 19.01 |
| ATOM | 2686 | CB  | ASN | A | 341 | 30.256 | 38.827 | 70.136 | 1.00 | 15.22 |
| ATOM | 2687 | CG  | ASN | A | 341 | 30.886 | 40.099 | 69.603 | 1.00 | 29.77 |
| ATOM | 2688 | OD1 | ASN | A | 341 | 31.197 | 40.172 | 68.416 | 1.00 | 60.07 |
| ATOM | 2689 | ND2 | ASN | A | 341 | 30.995 | 41.133 | 70.437 | 1.00 | 17.13 |
| ATOM | 2690 | N   | ALA | A | 342 | 29.908 | 36.511 | 72.229 | 1.00 | 11.92 |
| ATOM | 2691 | CA  | ALA | A | 342 | 29.065 | 35.487 | 72.804 | 1.00 | 12.85 |
| ATOM | 2692 | C   | ALA | A | 342 | 28.923 | 35.676 | 74.314 | 1.00 | 15.91 |
| ATOM | 2693 | O   | ALA | A | 342 | 27.832 | 35.578 | 74.884 | 1.00 | 14.84 |
| ATOM | 2694 | CB  | ALA | A | 342 | 29.614 | 34.099 | 72.492 | 1.00 | 12.26 |
| ATOM | 2695 | N   | LEU | A | 343 | 30.043 | 35.937 | 74.986 | 1.00 | 13.24 |
| ATOM | 2696 | CA  | LEU | A | 343 | 30.030 | 36.113 | 76.417 | 1.00 | 10.68 |
| ATOM | 2697 | C   | LEU | A | 343 | 29.264 | 37.372 | 76.748 | 1.00 | 14.78 |
| ATOM | 2698 | O   | LEU | A | 343 | 28.551 | 37.413 | 77.737 | 1.00 | 18.40 |
| ATOM | 2699 | CB  | LEU | A | 343 | 31.459 | 36.148 | 77.006 | 1.00 | 9.64  |
| ATOM | 2700 | CG  | LEU | A | 343 | 31.476 | 36.187 | 78.528 | 1.00 | 14.79 |
| ATOM | 2701 | CD1 | LEU | A | 343 | 30.680 | 35.010 | 79.105 | 1.00 | 11.42 |
| ATOM | 2702 | CD2 | LEU | A | 343 | 32.931 | 36.014 | 78.992 | 1.00 | 14.08 |
| ATOM | 2703 | N   | GLY | A | 344 | 29.420 | 38.440 | 75.953 | 1.00 | 10.89 |
| ATOM | 2704 | CA  | GLY | A | 344 | 28.648 | 39.658 | 76.253 | 1.00 | 10.09 |
| ATOM | 2705 | C   | GLY | A | 344 | 27.124 | 39.384 | 76.115 | 1.00 | 17.65 |
| ATOM | 2706 | O   | GLY | A | 344 | 26.321 | 39.969 | 76.838 | 1.00 | 17.82 |
| ATOM | 2707 | N   | GLY | A | 345 | 26.706 | 38.516 | 75.167 | 1.00 | 13.70 |
| ATOM | 2708 | CA  | GLY | A | 345 | 25.298 | 38.162 | 74.927 | 1.00 | 8.39  |
| ATOM | 2709 | C   | GLY | A | 345 | 24.753 | 37.490 | 76.190 | 1.00 | 13.97 |
| ATOM | 2710 | O   | GLY | A | 345 | 23.611 | 37.741 | 76.620 | 1.00 | 12.61 |
| ATOM | 2711 | N   | TRP | A | 346 | 25.592 | 36.634 | 76.814 | 1.00 | 13.97 |
| ATOM | 2712 | CA  | TRP | A | 346 | 25.230 | 35.929 | 78.059 | 1.00 | 9.72  |
| ATOM | 2713 | C   | TRP | A | 346 | 24.922 | 37.005 | 79.095 | 1.00 | 15.65 |
| ATOM | 2714 | O   | TRP | A | 346 | 23.975 | 36.947 | 79.906 | 1.00 | 12.16 |
| ATOM | 2715 | CB  | TRP | A | 346 | 26.367 | 34.981 | 78.555 | 1.00 | 8.14  |
| ATOM | 2716 | CG  | TRP | A | 346 | 25.958 | 34.282 | 79.835 | 1.00 | 10.60 |
| ATOM | 2717 | CD1 | TRP | A | 346 | 26.106 | 34.787 | 81.102 | 1.00 | 12.86 |
| ATOM | 2718 | CD2 | TRP | A | 346 | 25.267 | 33.009 | 80.004 | 1.00 | 11.80 |
| ATOM | 2719 | NE1 | TRP | A | 346 | 25.585 | 33.926 | 82.032 | 1.00 | 13.12 |
| ATOM | 2720 | CE2 | TRP | A | 346 | 25.065 | 32.806 | 81.394 | 1.00 | 16.02 |
| ATOM | 2721 | CE3 | TRP | A | 346 | 24.806 | 32.001 | 79.140 | 1.00 | 14.58 |
| ATOM | 2722 | CZ2 | TRP | A | 346 | 24.431 | 31.641 | 81.909 | 1.00 | 14.92 |
| ATOM | 2723 | CZ3 | TRP | A | 346 | 24.188 | 30.860 | 79.646 | 1.00 | 14.14 |
| ATOM | 2724 | CH2 | TRP | A | 346 | 23.982 | 30.685 | 81.027 | 1.00 | 14.57 |
| ATOM | 2725 | N   | GLY | A | 347 | 25.728 | 38.064 | 79.012 | 1.00 | 10.25 |
| ATOM | 2726 | CA  | GLY | A | 347 | 25.516 | 39.160 | 79.953 | 1.00 | 11.27 |
| ATOM | 2727 | C   | GLY | A | 347 | 24.171 | 39.838 | 79.758 | 1.00 | 11.91 |
| ATOM | 2728 | O   | GLY | A | 347 | 23.531 | 40.217 | 80.724 | 1.00 | 12.39 |
| ATOM | 2729 | N   | GLU | A | 348 | 23.789 | 40.049 | 78.500 | 1.00 | 13.80 |
| ATOM | 2730 | CA  | GLU | A | 348 | 22.502 | 40.674 | 78.185 | 1.00 | 11.62 |
| ATOM | 2731 | C   | GLU | A | 348 | 21.399 | 39.762 | 78.682 | 1.00 | 16.45 |
| ATOM | 2732 | O   | GLU | A | 348 | 20.381 | 40.234 | 79.211 | 1.00 | 14.72 |
| ATOM | 2733 | CB  | GLU | A | 348 | 22.401 | 40.992 | 76.683 | 1.00 | 11.49 |
| ATOM | 2734 | CG  | GLU | A | 348 | 23.434 | 42.056 | 76.317 | 1.00 | 12.72 |
| ATOM | 2735 | CD  | GLU | A | 348 | 23.027 | 43.349 | 76.970 | 1.00 | 29.34 |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 2736 | OE1 | GLU | A | 348 | 21.910 | 43.796 | 76.855 | 1.00 | 45.66 |
| ATOM | 2737 | OE2 | GLU | A | 348 | 23.939 | 43.872 | 77.746 | 1.00 | 21.11 |
| ATOM | 2738 | N   | LEU | A | 349 | 21.648 | 38.442 | 78.531 | 1.00 | 11.46 |
| ATOM | 2739 | CA  | LEU | A | 349 | 20.686 | 37.471 | 79.030 | 1.00 | 12.33 |
| ATOM | 2740 | C   | LEU | A | 349 | 20.538 | 37.591 | 80.565 | 1.00 | 17.72 |
| ATOM | 2741 | O   | LEU | A | 349 | 19.438 | 37.548 | 81.111 | 1.00 | 13.76 |
| ATOM | 2742 | CB  | LEU | A | 349 | 21.011 | 36.014 | 78.591 | 1.00 | 12.25 |
| ATOM | 2743 | CG  | LEU | A | 349 | 20.011 | 34.943 | 79.079 | 1.00 | 13.43 |
| ATOM | 2744 | CD1 | LEU | A | 349 | 18.665 | 35.153 | 78.379 | 1.00 | 9.66  |
| ATOM | 2745 | CD2 | LEU | A | 349 | 20.532 | 33.546 | 78.712 | 1.00 | 13.00 |
| ATOM | 2746 | N   | GLN | A | 350 | 21.631 | 37.719 | 81.301 | 1.00 | 12.48 |
| ATOM | 2747 | CA  | GLN | A | 350 | 21.524 | 37.864 | 82.738 | 1.00 | 8.81  |
| ATOM | 2748 | C   | GLN | A | 350 | 20.685 | 39.085 | 83.083 | 1.00 | 15.50 |
| ATOM | 2749 | O   | GLN | A | 350 | 19.876 | 39.083 | 84.015 | 1.00 | 18.35 |
| ATOM | 2750 | CB  | GLN | A | 350 | 22.929 | 38.135 | 83.300 | 1.00 | 12.42 |
| ATOM | 2751 | CG  | GLN | A | 350 | 23.810 | 36.867 | 83.324 | 1.00 | 13.26 |
| ATOM | 2752 | CD  | GLN | A | 350 | 25.238 | 37.162 | 83.789 | 1.00 | 25.25 |
| ATOM | 2753 | OE1 | GLN | A | 350 | 25.856 | 36.393 | 84.540 | 1.00 | 24.47 |
| ATOM | 2754 | NE2 | GLN | A | 350 | 25.770 | 38.303 | 83.383 | 1.00 | 17.04 |
| ATOM | 2755 | N   | ASN | A | 351 | 20.856 | 40.155 | 82.316 | 1.00 | 15.07 |
| ATOM | 2756 | CA  | ASN | A | 351 | 20.111 | 41.382 | 82.543 | 1.00 | 13.40 |
| ATOM | 2757 | C   | ASN | A | 351 | 18.641 | 41.166 | 82.291 | 1.00 | 15.52 |
| ATOM | 2758 | O   | ASN | A | 351 | 17.800 | 41.602 | 83.072 | 1.00 | 14.93 |
| ATOM | 2759 | CB  | ASN | A | 351 | 20.581 | 42.551 | 81.657 | 1.00 | 15.98 |
| ATOM | 2760 | CG  | ASN | A | 351 | 21.996 | 42.987 | 81.972 | 1.00 | 10.13 |
| ATOM | 2761 | OD1 | ASN | A | 351 | 22.615 | 42.513 | 82.928 | 1.00 | 16.52 |
| ATOM | 2762 | ND2 | ASN | A | 351 | 22.563 | 43.766 | 81.065 | 1.00 | 12.55 |
| ATOM | 2763 | N   | SER | A | 352 | 18.310 | 40.514 | 81.187 | 1.00 | 11.92 |
| ATOM | 2764 | CA  | SER | A | 352 | 16.888 | 40.272 | 80.893 | 1.00 | 12.49 |
| ATOM | 2765 | C   | SER | A | 352 | 16.167 | 39.437 | 81.959 | 1.00 | 16.90 |
| ATOM | 2766 | O   | SER | A | 352 | 15.015 | 39.650 | 82.332 | 1.00 | 15.33 |
| ATOM | 2767 | CB  | SER | A | 352 | 16.772 | 39.519 | 79.567 | 1.00 | 17.32 |
| ATOM | 2768 | OG  | SER | A | 352 | 16.959 | 40.434 | 78.526 | 1.00 | 24.23 |
| ATOM | 2769 | N   | VAL | A | 353 | 16.861 | 38.419 | 82.432 | 1.00 | 14.57 |
| ATOM | 2770 | CA  | VAL | A | 353 | 16.321 | 37.538 | 83.446 | 1.00 | 13.92 |
| ATOM | 2771 | C   | VAL | A | 353 | 16.163 | 38.312 | 84.734 | 1.00 | 20.86 |
| ATOM | 2772 | O   | VAL | A | 353 | 15.191 | 38.139 | 85.468 | 1.00 | 17.05 |
| ATOM | 2773 | CB  | VAL | A | 353 | 17.158 | 36.280 | 83.664 | 1.00 | 11.73 |
| ATOM | 2774 | CG1 | VAL | A | 353 | 16.794 | 35.472 | 84.932 | 1.00 | 9.84  |
| ATOM | 2775 | CG2 | VAL | A | 353 | 17.089 | 35.402 | 82.409 | 1.00 | 12.88 |
| ATOM | 2776 | N   | LYS | A | 354 | 17.112 | 39.198 | 84.995 | 1.00 | 14.12 |
| ATOM | 2777 | CA  | LYS | A | 354 | 17.002 | 39.913 | 86.238 | 1.00 | 12.36 |
| ATOM | 2778 | C   | LYS | A | 354 | 15.826 | 40.848 | 86.179 | 1.00 | 17.58 |
| ATOM | 2779 | O   | LYS | A | 354 | 15.072 | 41.024 | 87.109 | 1.00 | 19.87 |
| ATOM | 2780 | CB  | LYS | A | 354 | 18.298 | 40.637 | 86.571 | 1.00 | 17.00 |
| ATOM | 2781 | CG  | LYS | A | 354 | 18.143 | 41.562 | 87.760 | 1.00 | 23.68 |
| ATOM | 2782 | CD  | LYS | A | 354 | 19.434 | 42.305 | 88.057 | 1.00 | 46.34 |
| ATOM | 2783 | CE  | LYS | A | 354 | 19.458 | 43.018 | 89.409 | 1.00 | 67.61 |
| ATOM | 2784 | NZ  | LYS | A | 354 | 20.473 | 44.087 | 89.499 | 1.00 | 72.09 |
| ATOM | 2785 | N   | THR | A | 355 | 15.685 | 41.464 | 85.045 | 1.00 | 17.30 |
| ATOM | 2786 | CA  | THR | A | 355 | 14.634 | 42.423 | 84.776 | 1.00 | 19.03 |
| ATOM | 2787 | C   | THR | A | 355 | 13.239 | 41.788 | 84.894 | 1.00 | 24.56 |
| ATOM | 2788 | O   | THR | A | 355 | 12.375 | 42.258 | 85.644 | 1.00 | 21.41 |
| ATOM | 2789 | CB  | THR | A | 355 | 14.938 | 43.046 | 83.383 | 1.00 | 26.33 |
| ATOM | 2790 | OG1 | THR | A | 355 | 15.936 | 44.041 | 83.502 | 1.00 | 33.25 |
| ATOM | 2791 | CG2 | THR | A | 355 | 13.720 | 43.535 | 82.618 | 1.00 | 35.80 |
| ATOM | 2792 | N   | PHE | A | 356 | 12.986 | 40.698 | 84.173 | 1.00 | 15.72 |
| ATOM | 2793 | CA  | PHE | A | 356 | 11.685 | 40.084 | 84.266 | 1.00 | 13.01 |
| ATOM | 2794 | C   | PHE | A | 356 | 11.492 | 39.347 | 85.550 | 1.00 | 16.31 |
| ATOM | 2795 | O   | PHE | A | 356 | 10.364 | 39.197 | 85.974 | 1.00 | 17.60 |
| ATOM | 2796 | CB  | PHE | A | 356 | 11.633 | 38.916 | 83.282 | 1.00 | 14.64 |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 2797 | CG  | PHE | A | 356 | 11.306 | 39.389 | 81.925 | 1.00 | 20.28 |
| ATOM | 2798 | CD1 | PHE | A | 356 | 10.172 | 40.180 | 81.740 | 1.00 | 26.98 |
| ATOM | 2799 | CD2 | PHE | A | 356 | 12.119 | 39.030 | 80.848 | 1.00 | 25.24 |
| ATOM | 2800 | CE1 | PHE | A | 356 | 9.854  | 40.645 | 80.463 | 1.00 | 32.69 |
| ATOM | 2801 | CE2 | PHE | A | 356 | 11.801 | 39.480 | 79.568 | 1.00 | 32.46 |
| ATOM | 2802 | CZ  | PHE | A | 356 | 10.672 | 40.285 | 79.388 | 1.00 | 34.40 |
| ATOM | 2803 | N   | GLY | A | 357 | 12.567 | 38.773 | 86.080 | 1.00 | 13.33 |
| ATOM | 2804 | CA  | GLY | A | 357 | 12.484 | 37.898 | 87.250 | 1.00 | 13.08 |
| ATOM | 2805 | C   | GLY | A | 357 | 12.710 | 36.459 | 86.719 | 1.00 | 14.31 |
| ATOM | 2806 | O   | GLY | A | 357 | 12.203 | 36.080 | 85.639 | 1.00 | 15.86 |
| ATOM | 2807 | N   | GLU | A | 358 | 13.458 | 35.652 | 87.492 | 1.00 | 10.82 |
| ATOM | 2808 | CA  | GLU | A | 358 | 13.852 | 34.295 | 87.104 | 1.00 | 14.45 |
| ATOM | 2809 | C   | GLU | A | 358 | 12.748 | 33.275 | 86.946 | 1.00 | 17.31 |
| ATOM | 2810 | O   | GLU | A | 358 | 12.966 | 32.190 | 86.382 | 1.00 | 16.43 |
| ATOM | 2811 | CB  | GLU | A | 358 | 14.976 | 33.766 | 88.003 | 1.00 | 15.36 |
| ATOM | 2812 | CG  | GLU | A | 358 | 14.483 | 33.548 | 89.449 | 1.00 | 29.12 |
| ATOM | 2813 | CD  | GLU | A | 358 | 15.577 | 33.165 | 90.432 | 1.00 | 29.41 |
| ATOM | 2814 | OE1 | GLU | A | 358 | 16.737 | 32.999 | 90.104 | 1.00 | 53.87 |
| ATOM | 2815 | OE2 | GLU | A | 358 | 15.150 | 33.063 | 91.673 | 1.00 | 78.82 |
| ATOM | 2816 | N   | THR | A | 359 | 11.552 | 33.623 | 87.445 | 1.00 | 15.09 |
| ATOM | 2817 | CA  | THR | A | 359 | 10.397 | 32.715 | 87.319 | 1.00 | 14.57 |
| ATOM | 2818 | C   | THR | A | 359 | 9.370  | 33.195 | 86.297 | 1.00 | 18.20 |
| ATOM | 2819 | O   | THR | A | 359 | 8.308  | 32.602 | 86.161 | 1.00 | 17.32 |
| ATOM | 2820 | CB  | THR | A | 359 | 9.665  | 32.513 | 88.661 | 1.00 | 10.95 |
| ATOM | 2821 | OG1 | THR | A | 359 | 9.014  | 33.714 | 89.058 | 1.00 | 16.14 |
| ATOM | 2822 | CG2 | THR | A | 359 | 10.598 | 31.933 | 89.726 | 1.00 | 12.38 |
| ATOM | 2823 | N   | HIS | A | 360 | 9.704  | 34.267 | 85.600 | 1.00 | 13.00 |
| ATOM | 2824 | CA  | HIS | A | 360 | 8.838  | 34.886 | 84.648 | 1.00 | 13.62 |
| ATOM | 2825 | C   | HIS | A | 360 | 8.702  | 34.081 | 83.372 | 1.00 | 22.06 |
| ATOM | 2826 | O   | HIS | A | 360 | 9.701  | 33.663 | 82.770 | 1.00 | 18.40 |
| ATOM | 2827 | CB  | HIS | A | 360 | 9.369  | 36.276 | 84.298 | 1.00 | 14.44 |
| ATOM | 2828 | CG  | HIS | A | 360 | 8.321  | 37.043 | 83.556 | 1.00 | 16.43 |
| ATOM | 2829 | ND1 | HIS | A | 360 | 7.725  | 38.218 | 84.074 | 1.00 | 18.54 |
| ATOM | 2830 | CD2 | HIS | A | 360 | 7.765  | 36.779 | 82.349 | 1.00 | 13.02 |
| ATOM | 2831 | CE1 | HIS | A | 360 | 6.832  | 38.646 | 83.174 | 1.00 | 15.62 |
| ATOM | 2832 | NE2 | HIS | A | 360 | 6.848  | 37.781 | 82.139 | 1.00 | 17.56 |
| ATOM | 2833 | N   | PRO | A | 361 | 7.447  | 33.890 | 82.953 | 1.00 | 18.85 |
| ATOM | 2834 | CA  | PRO | A | 361 | 7.204  | 33.111 | 81.752 | 1.00 | 17.22 |
| ATOM | 2835 | C   | PRO | A | 361 | 7.871  | 33.616 | 80.481 | 1.00 | 18.11 |
| ATOM | 2836 | O   | PRO | A | 361 | 8.093  | 32.859 | 79.534 | 1.00 | 16.08 |
| ATOM | 2837 | CB  | PRO | A | 361 | 5.680  | 32.939 | 81.654 | 1.00 | 17.39 |
| ATOM | 2838 | CG  | PRO | A | 361 | 5.232  | 32.970 | 83.121 | 1.00 | 22.59 |
| ATOM | 2839 | CD  | PRO | A | 361 | 6.220  | 33.896 | 83.819 | 1.00 | 17.68 |
| ATOM | 2840 | N   | PHE | A | 362 | 8.192  | 34.899 | 80.434 | 1.00 | 13.89 |
| ATOM | 2841 | CA  | PHE | A | 362 | 8.822  | 35.408 | 79.237 | 1.00 | 15.98 |
| ATOM | 2842 | C   | PHE | A | 362 | 10.286 | 35.089 | 79.221 | 1.00 | 13.98 |
| ATOM | 2843 | O   | PHE | A | 362 | 10.926 | 35.501 | 78.277 | 1.00 | 14.94 |
| ATOM | 2844 | CB  | PHE | A | 362 | 8.690  | 36.921 | 79.035 | 1.00 | 19.97 |
| ATOM | 2845 | CG  | PHE | A | 362 | 7.273  | 37.416 | 78.899 | 1.00 | 23.23 |
| ATOM | 2846 | CD1 | PHE | A | 362 | 6.227  | 36.538 | 78.616 | 1.00 | 24.55 |
| ATOM | 2847 | CD2 | PHE | A | 362 | 6.998  | 38.782 | 79.021 | 1.00 | 27.19 |
| ATOM | 2848 | CE1 | PHE | A | 362 | 4.927  | 37.035 | 78.487 | 1.00 | 26.53 |
| ATOM | 2849 | CE2 | PHE | A | 362 | 5.704  | 39.298 | 78.891 | 1.00 | 31.58 |
| ATOM | 2850 | CZ  | PHE | A | 362 | 4.663  | 38.404 | 78.626 | 1.00 | 28.23 |
| ATOM | 2851 | N   | THR | A | 363 | 10.787 | 34.395 | 80.244 | 1.00 | 14.98 |
| ATOM | 2852 | CA  | THR | A | 363 | 12.209 | 33.992 | 80.288 | 1.00 | 12.84 |
| ATOM | 2853 | C   | THR | A | 363 | 12.446 | 32.567 | 79.724 | 1.00 | 19.07 |
| ATOM | 2854 | O   | THR | A | 363 | 13.562 | 32.031 | 79.682 | 1.00 | 15.98 |
| ATOM | 2855 | CB  | THR | A | 363 | 12.924 | 34.230 | 81.643 | 1.00 | 12.16 |
| ATOM | 2856 | OG1 | THR | A | 363 | 12.406 | 33.364 | 82.634 | 1.00 | 12.37 |
| ATOM | 2857 | CG2 | THR | A | 363 | 12.828 | 35.706 | 82.046 | 1.00 | 15.02 |



0012210-023699

|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 2858 | N   | LYS | A | 364 | 11.344 | 31.922 | 79.336 | 1.00 | 15.36 |
| ATOM | 2859 | CA  | LYS | A | 364 | 11.390 | 30.603 | 78.747 | 1.00 | 12.01 |
| ATOM | 2860 | C   | LYS | A | 364 | 11.762 | 30.792 | 77.276 | 1.00 | 15.28 |
| ATOM | 2861 | O   | LYS | A | 364 | 11.373 | 31.788 | 76.600 | 1.00 | 12.86 |
| ATOM | 2862 | CB  | LYS | A | 364 | 9.988  | 30.005 | 78.770 | 1.00 | 11.05 |
| ATOM | 2863 | CG  | LYS | A | 364 | 9.506  | 29.626 | 80.142 | 1.00 | 18.14 |
| ATOM | 2864 | CD  | LYS | A | 364 | 8.036  | 29.218 | 80.150 | 1.00 | 16.21 |
| ATOM | 2865 | CE  | LYS | A | 364 | 7.664  | 28.728 | 81.534 | 1.00 | 29.65 |
| ATOM | 2866 | NZ  | LYS | A | 364 | 6.221  | 28.541 | 81.736 | 1.00 | 39.48 |
| ATOM | 2867 | N   | LEU | A | 365 | 12.474 | 29.806 | 76.720 | 1.00 | 13.94 |
| ATOM | 2868 | CA  | LEU | A | 365 | 12.885 | 29.872 | 75.325 | 1.00 | 12.51 |
| ATOM | 2869 | C   | LEU | A | 365 | 11.671 | 29.766 | 74.388 | 1.00 | 18.38 |
| ATOM | 2870 | O   | LEU | A | 365 | 11.491 | 30.548 | 73.436 | 1.00 | 17.81 |
| ATOM | 2871 | CB  | LEU | A | 365 | 13.926 | 28.767 | 75.037 | 1.00 | 13.31 |
| ATOM | 2872 | CG  | LEU | A | 365 | 14.542 | 28.857 | 73.653 | 1.00 | 18.68 |
| ATOM | 2873 | CD1 | LEU | A | 365 | 15.219 | 30.203 | 73.489 | 1.00 | 19.46 |
| ATOM | 2874 | CD2 | LEU | A | 365 | 15.612 | 27.777 | 73.545 | 1.00 | 19.36 |
| ATOM | 2875 | N   | VAL | A | 366 | 10.805 | 28.804 | 74.685 | 1.00 | 15.92 |
| ATOM | 2876 | CA  | VAL | A | 366 | 9.534  | 28.572 | 73.964 | 1.00 | 18.17 |
| ATOM | 2877 | C   | VAL | A | 366 | 8.411  | 29.193 | 74.832 | 1.00 | 19.02 |
| ATOM | 2878 | O   | VAL | A | 366 | 8.188  | 28.759 | 75.953 | 1.00 | 15.50 |
| ATOM | 2879 | CB  | VAL | A | 366 | 9.276  | 27.091 | 73.587 | 1.00 | 17.55 |
| ATOM | 2880 | CG1 | VAL | A | 366 | 7.985  | 26.938 | 72.761 | 1.00 | 13.93 |
| ATOM | 2881 | CG2 | VAL | A | 366 | 10.488 | 26.522 | 72.828 | 1.00 | 15.55 |
| ATOM | 2882 | N   | VAL | A | 367 | 7.724  | 30.226 | 74.348 | 1.00 | 15.38 |
| ATOM | 2883 | CA  | VAL | A | 367 | 6.725  | 30.907 | 75.166 | 1.00 | 14.70 |
| ATOM | 2884 | C   | VAL | A | 367 | 5.318  | 30.654 | 74.723 | 1.00 | 22.22 |
| ATOM | 2885 | O   | VAL | A | 367 | 5.145  | 30.064 | 73.683 | 1.00 | 21.51 |
| ATOM | 2886 | CB  | VAL | A | 367 | 6.946  | 32.396 | 75.034 | 1.00 | 17.48 |
| ATOM | 2887 | CG1 | VAL | A | 367 | 8.305  | 32.742 | 75.633 | 1.00 | 17.07 |
| ATOM | 2888 | CG2 | VAL | A | 367 | 6.874  | 32.793 | 73.566 | 1.00 | 15.29 |
| ATOM | 2889 | N   | ASP | A | 368 | 4.331  | 31.134 | 75.471 | 1.00 | 17.48 |
| ATOM | 2890 | CA  | ASP | A | 368 | 2.937  | 30.940 | 75.054 | 1.00 | 16.38 |
| ATOM | 2891 | C   | ASP | A | 368 | 2.362  | 32.335 | 74.997 | 1.00 | 14.53 |
| ATOM | 2892 | O   | ASP | A | 368 | 2.198  | 32.991 | 75.998 | 1.00 | 18.37 |
| ATOM | 2893 | CB  | ASP | A | 368 | 2.181  | 30.036 | 76.049 | 1.00 | 17.68 |
| ATOM | 2894 | CG  | ASP | A | 368 | 0.683  | 29.999 | 75.796 | 1.00 | 25.53 |
| ATOM | 2895 | OD1 | ASP | A | 368 | 0.115  | 30.610 | 74.927 | 1.00 | 17.63 |
| ATOM | 2896 | OD2 | ASP | A | 368 | 0.047  | 29.214 | 76.601 | 1.00 | 31.38 |
| ATOM | 2897 | N   | LEU | A | 369 | 2.161  | 32.859 | 73.829 | 1.00 | 10.10 |
| ATOM | 2898 | CA  | LEU | A | 369 | 1.697  | 34.212 | 73.698 | 1.00 | 12.48 |
| ATOM | 2899 | C   | LEU | A | 369 | 0.215  | 34.381 | 73.668 | 1.00 | 18.80 |
| ATOM | 2900 | O   | LEU | A | 369 | -0.276 | 35.378 | 73.147 | 1.00 | 21.46 |
| ATOM | 2901 | CB  | LEU | A | 369 | 2.274  | 34.974 | 72.500 | 1.00 | 10.77 |
| ATOM | 2902 | CG  | LEU | A | 369 | 3.779  | 35.129 | 72.552 | 1.00 | 17.85 |
| ATOM | 2903 | CD1 | LEU | A | 369 | 4.256  | 35.435 | 71.127 | 1.00 | 16.11 |
| ATOM | 2904 | CD2 | LEU | A | 369 | 4.076  | 36.290 | 73.493 | 1.00 | 16.09 |
| ATOM | 2905 | N   | THR | A | 370 | -0.484 | 33.422 | 74.207 | 1.00 | 18.13 |
| ATOM | 2906 | CA  | THR | A | 370 | -1.922 | 33.603 | 74.226 | 1.00 | 19.34 |
| ATOM | 2907 | C   | THR | A | 370 | -2.259 | 34.856 | 75.052 | 1.00 | 24.31 |
| ATOM | 2908 | O   | THR | A | 370 | -1.890 | 35.048 | 76.218 | 1.00 | 22.17 |
| ATOM | 2909 | CB  | THR | A | 370 | -2.558 | 32.439 | 74.994 | 1.00 | 31.44 |
| ATOM | 2910 | OG1 | THR | A | 370 | -2.383 | 31.226 | 74.291 | 1.00 | 25.88 |
| ATOM | 2911 | CG2 | THR | A | 370 | -4.020 | 32.785 | 75.234 | 1.00 | 26.93 |
| ATOM | 2912 | N   | ASP | A | 371 | -3.003 | 35.742 | 74.449 | 1.00 | 22.55 |
| ATOM | 2913 | CA  | ASP | A | 371 | -3.367 | 36.940 | 75.169 | 1.00 | 23.57 |
| ATOM | 2914 | C   | ASP | A | 371 | -2.254 | 37.904 | 75.464 | 1.00 | 24.80 |
| ATOM | 2915 | O   | ASP | A | 371 | -2.491 | 38.846 | 76.176 | 1.00 | 21.58 |
| ATOM | 2916 | CB  | ASP | A | 371 | -4.191 | 36.676 | 76.420 | 1.00 | 26.84 |
| ATOM | 2917 | CG  | ASP | A | 371 | -5.528 | 36.132 | 75.994 | 1.00 | 39.22 |
| ATOM | 2918 | OD1 | ASP | A | 371 | -6.111 | 36.460 | 74.949 | 1.00 | 32.59 |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 2919 | OD2 | ASP | A | 371 | -5.951 | 35.237 | 76.850 | 1.00 | 41.05 |
| ATOM | 2920 | N   | ILE | A | 372 | -1.084 | 37.719 | 74.889 | 1.00 | 20.31 |
| ATOM | 2921 | CA  | ILE | A | 372 | -0.009 | 38.663 | 75.120 | 1.00 | 17.55 |
| ATOM | 2922 | C   | ILE | A | 372 | 0.375  | 39.330 | 73.822 | 1.00 | 19.77 |
| ATOM | 2923 | O   | ILE | A | 372 | 0.553  | 38.641 | 72.818 | 1.00 | 22.17 |
| ATOM | 2924 | CB  | ILE | A | 372 | 1.249  | 37.911 | 75.480 | 1.00 | 20.80 |
| ATOM | 2925 | CG1 | ILE | A | 372 | 1.016  | 36.973 | 76.645 | 1.00 | 22.62 |
| ATOM | 2926 | CG2 | ILE | A | 372 | 2.392  | 38.904 | 75.707 | 1.00 | 22.69 |
| ATOM | 2927 | CD1 | ILE | A | 372 | 0.374  | 37.712 | 77.794 | 1.00 | 32.92 |
| ATOM | 2928 | N   | ASP | A | 373 | 0.560  | 40.636 | 73.857 | 1.00 | 14.79 |
| ATOM | 2929 | CA  | ASP | A | 373 | 0.958  | 41.385 | 72.693 | 1.00 | 14.17 |
| ATOM | 2930 | C   | ASP | A | 373 | 2.445  | 41.160 | 72.485 | 1.00 | 21.76 |
| ATOM | 2931 | O   | ASP | A | 373 | 3.280  | 41.384 | 73.355 | 1.00 | 21.72 |
| ATOM | 2932 | CB  | ASP | A | 373 | 0.717  | 42.882 | 72.934 | 1.00 | 15.14 |
| ATOM | 2933 | CG  | ASP | A | 373 | 1.247  | 43.773 | 71.829 | 1.00 | 21.68 |
| ATOM | 2934 | OD1 | ASP | A | 373 | 2.004  | 43.399 | 70.933 | 1.00 | 23.88 |
| ATOM | 2935 | OD2 | ASP | A | 373 | 0.769  | 45.005 | 71.893 | 1.00 | 22.14 |
| ATOM | 2936 | N   | PRO | A | 374 | 2.810  | 40.719 | 71.305 | 1.00 | 21.82 |
| ATOM | 2937 | CA  | PRO | A | 374 | 4.210  | 40.450 | 71.050 | 1.00 | 21.09 |
| ATOM | 2938 | C   | PRO | A | 374 | 5.149  | 41.600 | 71.350 | 1.00 | 19.90 |
| ATOM | 2939 | O   | PRO | A | 374 | 6.240  | 41.371 | 71.873 | 1.00 | 14.86 |
| ATOM | 2940 | CB  | PRO | A | 374 | 4.312  | 39.943 | 69.607 | 1.00 | 23.86 |
| ATOM | 2941 | CG  | PRO | A | 374 | 2.896  | 39.591 | 69.183 | 1.00 | 24.47 |
| ATOM | 2942 | CD  | PRO | A | 374 | 1.967  | 40.317 | 70.149 | 1.00 | 22.40 |
| ATOM | 2943 | N   | ASP | A | 375 | 4.722  | 42.819 | 71.007 | 1.00 | 14.82 |
| ATOM | 2944 | CA  | ASP | A | 375 | 5.537  | 44.022 | 71.250 | 1.00 | 16.55 |
| ATOM | 2945 | C   | ASP | A | 375 | 5.870  | 44.193 | 72.728 | 1.00 | 20.20 |
| ATOM | 2946 | O   | ASP | A | 375 | 6.896  | 44.725 | 73.140 | 1.00 | 19.90 |
| ATOM | 2947 | CB  | ASP | A | 375 | 4.811  | 45.273 | 70.724 | 1.00 | 15.07 |
| ATOM | 2948 | CG  | ASP | A | 375 | 4.971  | 45.315 | 69.240 | 1.00 | 18.22 |
| ATOM | 2949 | OD1 | ASP | A | 375 | 5.933  | 44.823 | 68.667 | 1.00 | 18.62 |
| ATOM | 2950 | OD2 | ASP | A | 375 | 3.980  | 45.894 | 68.637 | 1.00 | 21.94 |
| ATOM | 2951 | N   | VAL | A | 376 | 4.952  | 43.710 | 73.532 | 1.00 | 17.46 |
| ATOM | 2952 | CA  | VAL | A | 376 | 5.064  | 43.756 | 74.968 | 1.00 | 17.12 |
| ATOM | 2953 | C   | VAL | A | 376 | 5.930  | 42.629 | 75.532 | 1.00 | 22.81 |
| ATOM | 2954 | O   | VAL | A | 376 | 6.634  | 42.825 | 76.514 | 1.00 | 23.05 |
| ATOM | 2955 | CB  | VAL | A | 376 | 3.686  | 43.683 | 75.601 | 1.00 | 19.84 |
| ATOM | 2956 | CG1 | VAL | A | 376 | 3.841  | 43.374 | 77.085 | 1.00 | 21.03 |
| ATOM | 2957 | CG2 | VAL | A | 376 | 2.950  | 45.006 | 75.445 | 1.00 | 15.99 |
| ATOM | 2958 | N   | ALA | A | 377 | 5.896  | 41.436 | 74.950 | 1.00 | 16.51 |
| ATOM | 2959 | CA  | ALA | A | 377 | 6.711  | 40.369 | 75.484 | 1.00 | 15.14 |
| ATOM | 2960 | C   | ALA | A | 377 | 8.136  | 40.459 | 74.987 | 1.00 | 16.36 |
| ATOM | 2961 | O   | ALA | A | 377 | 9.037  | 39.827 | 75.498 | 1.00 | 13.72 |
| ATOM | 2962 |     |     |   |     |        |        |        |      |       |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 2980 | OG  | SER | A | 379 | 13.035 | 38.846 | 76.268 | 1.00 | 14.44 |
| ATOM | 2981 | N   | SER | A | 380 | 15.431 | 40.094 | 75.019 | 1.00 | 13.34 |
| ATOM | 2982 | CA  | SER | A | 380 | 16.705 | 39.480 | 74.595 | 1.00 | 13.12 |
| ATOM | 2983 | C   | SER | A | 380 | 16.734 | 37.989 | 74.811 | 1.00 | 13.76 |
| ATOM | 2984 | O   | SER | A | 380 | 17.705 | 37.336 | 74.470 | 1.00 | 15.40 |
| ATOM | 2985 | CB  | SER | A | 380 | 17.864 | 40.053 | 75.421 | 1.00 | 12.15 |
| ATOM | 2986 | OG  | SER | A | 380 | 17.883 | 41.443 | 75.162 | 1.00 | 18.31 |
| ATOM | 2987 | N   | VAL | A | 381 | 15.685 | 37.472 | 75.444 | 1.00 | 10.45 |
| ATOM | 2988 | CA  | VAL | A | 381 | 15.613 | 36.070 | 75.778 | 1.00 | 10.90 |
| ATOM | 2989 | C   | VAL | A | 381 | 15.709 | 35.177 | 74.561 | 1.00 | 15.64 |
| ATOM | 2990 | O   | VAL | A | 381 | 16.547 | 34.295 | 74.468 | 1.00 | 17.11 |
| ATOM | 2991 | CB  | VAL | A | 381 | 14.384 | 35.734 | 76.636 | 1.00 | 12.01 |
| ATOM | 2992 | CG1 | VAL | A | 381 | 14.269 | 34.234 | 76.861 | 1.00 | 12.07 |
| ATOM | 2993 | CG2 | VAL | A | 381 | 14.410 | 36.468 | 77.980 | 1.00 | 9.45  |
| ATOM | 2994 | N   | PRO | A | 382 | 14.832 | 35.347 | 73.603 | 1.00 | 12.68 |
| ATOM | 2995 | CA  | PRO | A | 382 | 14.939 | 34.427 | 72.488 | 1.00 | 11.41 |
| ATOM | 2996 | C   | PRO | A | 382 | 16.300 | 34.551 | 71.794 | 1.00 | 17.91 |
| ATOM | 2997 | O   | PRO | A | 382 | 16.830 | 33.564 | 71.249 | 1.00 | 16.29 |
| ATOM | 2998 | CB  | PRO | A | 382 | 13.817 | 34.802 | 71.513 | 1.00 | 11.39 |
| ATOM | 2999 | CG  | PRO | A | 382 | 13.328 | 36.176 | 71.947 | 1.00 | 14.03 |
| ATOM | 3000 | CD  | PRO | A | 382 | 13.778 | 36.366 | 73.378 | 1.00 | 10.32 |
| ATOM | 3001 | N   | TYR | A | 383 | 16.835 | 35.791 | 71.761 | 1.00 | 11.66 |
| ATOM | 3002 | CA  | TYR | A | 383 | 18.106 | 36.045 | 71.127 | 1.00 | 11.53 |
| ATOM | 3003 | C   | TYR | A | 383 | 19.229 | 35.291 | 71.821 | 1.00 | 17.48 |
| ATOM | 3004 | O   | TYR | A | 383 | 19.975 | 34.554 | 71.192 | 1.00 | 13.36 |
| ATOM | 3005 | CB  | TYR | A | 383 | 18.443 | 37.560 | 71.238 | 1.00 | 12.85 |
| ATOM | 3006 | CG  | TYR | A | 383 | 17.598 | 38.417 | 70.335 | 1.00 | 14.70 |
| ATOM | 3007 | CD1 | TYR | A | 383 | 16.309 | 38.809 | 70.707 | 1.00 | 16.40 |
| ATOM | 3008 | CD2 | TYR | A | 383 | 18.069 | 38.790 | 69.073 | 1.00 | 13.38 |
| ATOM | 3009 | CE1 | TYR | A | 383 | 15.536 | 39.577 | 69.832 | 1.00 | 15.57 |
| ATOM | 3010 | CE2 | TYR | A | 383 | 17.318 | 39.560 | 68.187 | 1.00 | 10.16 |
| ATOM | 3011 | CZ  | TYR | A | 383 | 16.039 | 39.947 | 68.582 | 1.00 | 14.31 |
| ATOM | 3012 | OH  | TYR | A | 383 | 15.280 | 40.713 | 67.728 | 1.00 | 12.64 |
| ATOM | 3013 | N   | GLU | A | 384 | 19.335 | 35.529 | 73.134 | 1.00 | 12.00 |
| ATOM | 3014 | CA  | GLU | A | 384 | 20.409 | 35.067 | 73.989 | 1.00 | 10.21 |
| ATOM | 3015 | C   | GLU | A | 384 | 20.251 | 33.701 | 74.605 | 1.00 | 15.22 |
| ATOM | 3016 | O   | GLU | A | 384 | 21.228 | 32.952 | 74.692 | 1.00 | 12.89 |
| ATOM | 3017 | CB  | GLU | A | 384 | 20.888 | 36.205 | 74.899 | 1.00 | 9.54  |
| ATOM | 3018 | CG  | GLU | A | 384 | 21.207 | 37.468 | 74.056 | 1.00 | 7.64  |
| ATOM | 3019 | CD  | GLU | A | 384 | 22.497 | 37.277 | 73.260 | 1.00 | 19.43 |
| ATOM | 3020 | OE1 | GLU | A | 384 | 23.237 | 36.310 | 73.331 | 1.00 | 15.97 |
| ATOM | 3021 | OE2 | GLU | A | 384 | 22.779 | 38.260 | 72.480 | 1.00 | 11.96 |
| ATOM | 3022 | N   | LYS | A | 385 | 19.036 | 33.345 | 75.034 | 1.00 | 12.07 |
| ATOM | 3023 | CA  | LYS | A | 385 | 18.898 | 31.984 | 75.533 | 1.00 | 13.42 |
| ATOM | 3024 | C   | LYS | A | 385 | 19.015 | 31.052 | 74.294 | 1.00 | 16.08 |
| ATOM | 3025 | O   | LYS | A | 385 | 19.593 | 29.947 | 74.359 | 1.00 | 13.01 |
| ATOM | 3026 | CB  | LYS | A | 385 | 17.623 | 31.742 | 76.350 | 1.00 | 12.55 |
| ATOM | 3027 | CG  | LYS | A | 385 | 17.554 | 30.302 | 76.839 | 1.00 | 14.13 |
| ATOM | 3028 | CD  | LYS | A | 385 | 16.371 | 29.987 | 77.750 | 1.00 | 11.06 |
| ATOM | 3029 | CE  | LYS | A | 385 | 16.360 | 30.692 | 79.099 | 1.00 | 12.13 |
| ATOM | 3030 | NZ  | LYS | A | 385 | 15.359 | 30.132 | 80.029 | 1.00 | 11.47 |
| ATOM | 3031 | N   | GLY | A | 386 | 18.477 | 31.533 | 73.138 | 1.00 | 11.14 |
| ATOM | 3032 | CA  | GLY | A | 386 | 18.521 | 30.792 | 71.864 | 1.00 | 9.75  |
| ATOM | 3033 | C   | GLY | A | 386 | 19.974 | 30.567 | 71.409 | 1.00 | 16.73 |
| ATOM | 3034 | O   | GLY | A | 386 | 20.417 | 29.446 | 71.100 | 1.00 | 13.12 |
| ATOM | 3035 | N   | PHE | A | 387 | 20.747 | 31.663 | 71.383 | 1.00 | 15.76 |
| ATOM | 3036 | CA  | PHE | A | 387 | 22.155 | 31.620 | 71.013 | 1.00 | 13.70 |
| ATOM | 3037 | C   | PHE | A | 387 | 22.926 | 30.744 | 71.982 | 1.00 | 17.51 |
| ATOM | 3038 | O   | PHE | A | 387 | 23.763 | 29.955 | 71.563 | 1.00 | 14.54 |
| ATOM | 3039 | CB  | PHE | A | 387 | 22.846 | 32.992 | 70.918 | 1.00 | 13.42 |
| ATOM | 3040 | CG  | PHE | A | 387 | 24.350 | 32.820 | 70.816 | 1.00 | 12.26 |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 3041 | CD1 | PHE | A | 387 | 24.963 | 32.588 | 69.582 | 1.00 | 11.34 |
| ATOM | 3042 | CD2 | PHE | A | 387 | 25.170 | 32.869 | 71.944 | 1.00 | 14.36 |
| ATOM | 3043 | CE1 | PHE | A | 387 | 26.346 | 32.422 | 69.468 | 1.00 | 12.53 |
| ATOM | 3044 | CE2 | PHE | A | 387 | 26.558 | 32.693 | 71.864 | 1.00 | 12.76 |
| ATOM | 3045 | CZ  | PHE | A | 387 | 27.141 | 32.454 | 70.618 | 1.00 | 8.96  |
| ATOM | 3046 | N   | ALA | A | 388 | 22.620 | 30.836 | 73.284 | 1.00 | 15.35 |
| ATOM | 3047 | CA  | ALA | A | 388 | 23.344 | 30.017 | 74.240 | 1.00 | 12.20 |
| ATOM | 3048 | C   | ALA | A | 388 | 23.084 | 28.552 | 74.014 | 1.00 | 15.51 |
| ATOM | 3049 | O   | ALA | A | 388 | 23.973 | 27.717 | 74.125 | 1.00 | 16.33 |
| ATOM | 3050 | CB  | ALA | A | 388 | 22.970 | 30.429 | 75.655 | 1.00 | 13.75 |
| ATOM | 3051 | N   | LEU | A | 389 | 21.843 | 28.209 | 73.701 | 1.00 | 12.77 |
| ATOM | 3052 | CA  | LEU | A | 389 | 21.542 | 26.793 | 73.446 | 1.00 | 13.17 |
| ATOM | 3053 | C   | LEU | A | 389 | 22.382 | 26.286 | 72.266 | 1.00 | 20.08 |
| ATOM | 3054 | O   | LEU | A | 389 | 23.030 | 25.214 | 72.312 | 1.00 | 16.85 |
| ATOM | 3055 | CB  | LEU | A | 389 | 20.065 | 26.657 | 73.061 | 1.00 | 9.51  |
| ATOM | 3056 | CG  | LEU | A | 389 | 19.639 | 25.263 | 72.656 | 1.00 | 16.80 |
| ATOM | 3057 | CD1 | LEU | A | 389 | 20.089 | 24.265 | 73.719 | 1.00 | 16.85 |
| ATOM | 3058 | CD2 | LEU | A | 389 | 18.119 | 25.247 | 72.538 | 1.00 | 12.75 |
| ATOM | 3059 | N   | LEU | A | 390 | 22.374 | 27.059 | 71.172 | 1.00 | 11.37 |
| ATOM | 3060 | CA  | LEU | A | 390 | 23.140 | 26.650 | 69.998 | 1.00 | 9.78  |
| ATOM | 3061 | C   | LEU | A | 390 | 24.651 | 26.539 | 70.251 | 1.00 | 19.70 |
| ATOM | 3062 | O   | LEU | A | 390 | 25.305 | 25.609 | 69.745 | 1.00 | 18.74 |
| ATOM | 3063 | CB  | LEU | A | 390 | 22.887 | 27.525 | 68.764 | 1.00 | 9.94  |
| ATOM | 3064 | CG  | LEU | A | 390 | 21.402 | 27.590 | 68.367 | 1.00 | 14.32 |
| ATOM | 3065 | CD1 | LEU | A | 390 | 21.153 | 28.632 | 67.257 | 1.00 | 14.04 |
| ATOM | 3066 | CD2 | LEU | A | 390 | 20.902 | 26.209 | 67.923 | 1.00 | 14.70 |
| ATOM | 3067 | N   | PHE | A | 391 | 25.205 | 27.490 | 71.026 | 1.00 | 12.66 |
| ATOM | 3068 | CA  | PHE | A | 391 | 26.635 | 27.538 | 71.333 | 1.00 | 13.86 |
| ATOM | 3069 | C   | PHE | A | 391 | 27.053 | 26.343 | 72.147 | 1.00 | 17.87 |
| ATOM | 3070 | O   | PHE | A | 391 | 28.104 | 25.733 | 71.983 | 1.00 | 18.52 |
| ATOM | 3071 | CB  | PHE | A | 391 | 26.964 | 28.806 | 72.105 | 1.00 | 14.47 |
| ATOM | 3072 | CG  | PHE | A | 391 | 28.437 | 29.179 | 72.101 | 1.00 | 18.51 |
| ATOM | 3073 | CD1 | PHE | A | 391 | 29.237 | 28.996 | 70.973 | 1.00 | 18.55 |
| ATOM | 3074 | CD2 | PHE | A | 391 | 29.030 | 29.748 | 73.233 | 1.00 | 18.59 |
| ATOM | 3075 | CE1 | PHE | A | 391 | 30.571 | 29.402 | 70.966 | 1.00 | 15.73 |
| ATOM | 3076 | CE2 | PHE | A | 391 | 30.373 | 30.137 | 73.252 | 1.00 | 18.49 |
| ATOM | 3077 | CZ  | PHE | A | 391 | 31.148 | 29.954 | 72.109 | 1.00 | 15.63 |
| ATOM | 3078 | N   | TYR | A | 392 | 26.148 | 26.008 | 73.039 | 1.00 | 16.91 |
| ATOM | 3079 | CA  | TYR | A | 392 | 26.315 | 24.893 | 73.944 | 1.00 | 17.78 |
| ATOM | 3080 | C   | TYR | A | 392 | 26.288 | 23.570 | 73.175 | 1.00 | 19.46 |
| ATOM | 3081 | O   | TYR | A | 392 | 27.095 | 22.666 | 73.388 | 1.00 | 18.21 |
| ATOM | 3082 | CB  | TYR | A | 392 | 25.243 | 25.000 | 75.049 | 1.00 | 15.50 |
| ATOM | 3083 | CG  | TYR | A | 392 | 24.    |        |        |      |       |



|      |      |     |     |   |     |        |        |        |      |        |
|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
| ATOM | 3102 | CB  | GLU | A | 394 | 28.434 | 24.745 | 68.776 | 1.00 | 17.59  |
| ATOM | 3103 | CG  | GLU | A | 394 | 29.903 | 24.871 | 68.320 | 1.00 | 23.24  |
| ATOM | 3104 | CD  | GLU | A | 394 | 30.332 | 26.300 | 68.152 | 1.00 | 32.12  |
| ATOM | 3105 | OE1 | GLU | A | 394 | 29.709 | 27.146 | 67.532 | 1.00 | 23.57  |
| ATOM | 3106 | OE2 | GLU | A | 394 | 31.480 | 26.547 | 68.714 | 1.00 | 26.27  |
| ATOM | 3107 | N   | GLN | A | 395 | 29.410 | 23.127 | 71.183 | 1.00 | 16.99  |
| ATOM | 3108 | CA  | GLN | A | 395 | 30.462 | 22.610 | 72.030 | 1.00 | 17.56  |
| ATOM | 3109 | C   | GLN | A | 395 | 30.293 | 21.127 | 72.360 | 1.00 | 23.89  |
| ATOM | 3110 | O   | GLN | A | 395 | 31.258 | 20.359 | 72.421 | 1.00 | 24.66  |
| ATOM | 3111 | CB  | GLN | A | 395 | 30.725 | 23.461 | 73.318 | 1.00 | 17.71  |
| ATOM | 3112 | CG  | GLN | A | 395 | 31.195 | 24.888 | 72.918 | 1.00 | 17.45  |
| ATOM | 3113 | CD  | GLN | A | 395 | 31.354 | 25.851 | 74.081 | 1.00 | 21.98  |
| ATOM | 3114 | OE1 | GLN | A | 395 | 30.986 | 25.584 | 75.224 | 1.00 | 16.80  |
| ATOM | 3115 | NE2 | GLN | A | 395 | 31.943 | 26.985 | 73.776 | 1.00 | 16.78  |
| ATOM | 3116 | N   | LEU | A | 396 | 29.058 | 20.706 | 72.588 | 1.00 | 21.86  |
| ATOM | 3117 | CA  | LEU | A | 396 | 28.767 | 19.330 | 72.932 | 1.00 | 20.27  |
| ATOM | 3118 | C   | LEU | A | 396 | 28.936 | 18.387 | 71.744 | 1.00 | 22.03  |
| ATOM | 3119 | O   | LEU | A | 396 | 29.381 | 17.260 | 71.857 | 1.00 | 25.07  |
| ATOM | 3120 | CB  | LEU | A | 396 | 27.315 | 19.276 | 73.441 | 1.00 | 18.56  |
| ATOM | 3121 | CG  | LEU | A | 396 | 26.852 | 17.960 | 73.994 | 1.00 | 22.66  |
| ATOM | 3122 | CD1 | LEU | A | 396 | 27.493 | 17.780 | 75.354 | 1.00 | 25.52  |
| ATOM | 3123 | CD2 | LEU | A | 396 | 25.340 | 18.045 | 74.179 | 1.00 | 17.79  |
| ATOM | 3124 | N   | LEU | A | 397 | 28.575 | 18.831 | 70.579 | 1.00 | 15.28  |
| ATOM | 3125 | CA  | LEU | A | 397 | 28.603 | 17.939 | 69.433 | 1.00 | 16.80  |
| ATOM | 3126 | C   | LEU | A | 397 | 29.846 | 17.946 | 68.565 | 1.00 | 26.85  |
| ATOM | 3127 | O   | LEU | A | 397 | 29.864 | 17.399 | 67.458 | 1.00 | 29.08  |
| ATOM | 3128 | CB  | LEU | A | 397 | 27.371 | 18.242 | 68.552 | 1.00 | 15.51  |
| ATOM | 3129 | CG  | LEU | A | 397 | 26.013 | 18.018 | 69.261 | 1.00 | 20.96  |
| ATOM | 3130 | CD1 | LEU | A | 397 | 24.874 | 18.717 | 68.501 | 1.00 | 19.35  |
| ATOM | 3131 | CD2 | LEU | A | 397 | 25.692 | 16.536 | 69.461 | 1.00 | 19.12  |
| ATOM | 3132 | N   | GLY | A | 398 | 30.901 | 18.598 | 68.985 | 1.00 | 24.55  |
| ATOM | 3133 | CA  | GLY | A | 398 | 32.006 | 18.516 | 68.076 | 1.00 | 27.19  |
| ATOM | 3134 | C   | GLY | A | 398 | 32.648 | 19.794 | 67.598 | 1.00 | 29.41  |
| ATOM | 3135 | O   | GLY | A | 398 | 33.743 | 19.713 | 67.048 | 1.00 | 30.13  |
| ATOM | 3136 | N   | GLY | A | 399 | 32.020 | 20.951 | 67.752 | 1.00 | 19.25  |
| ATOM | 3137 | CA  | GLY | A | 399 | 32.700 | 22.143 | 67.291 | 1.00 | 16.50  |
| ATOM | 3138 | C   | GLY | A | 399 | 31.937 | 22.850 | 66.212 | 1.00 | 15.03  |
| ATOM | 3139 | O   | GLY | A | 399 | 30.976 | 22.315 | 65.694 | 1.00 | 17.49  |
| ATOM | 3140 | N   | PRO | A | 400 | 32.397 | 24.045 | 65.870 | 1.00 | 21.52  |
| ATOM | 3141 | CA  | PRO | A | 400 | 31.758 | 24.918 | 64.909 | 1.00 | 21.69  |
| ATOM | 3142 | C   | PRO | A | 400 | 31.599 | 24.312 | 63.552 | 1.00 | 29.85  |
| ATOM | 3143 | O   | PRO | A | 400 | 30.540 | 24.433 | 62.921 | 1.00 | 24.28  |
| ATOM | 3144 | CB  | PRO | A | 400 | 32.574 | 26.210 | 64.802 | 1.00 | 21.33  |
| ATOM | 3145 | CG  | PRO | A | 400 | 33.868 | 25.949 | 65.552 | 1.00 | 27.07  |
| ATOM | 3146 | CD  | PRO | A | 400 | 33.698 | 24.635 | 66.306 | 1.00 | 25.67  |
| ATOM | 3147 | N   | GLU | A | 401 | 32.679 | 23.674 | 63.128 | 1.00 | 28.84  |
| ATOM | 3148 | CA  | GLU | A | 401 | 32.630 | 23.048 | 61.831 | 1.00 | 30.42  |
| ATOM | 3149 | C   | GLU | A | 401 | 31.491 | 22.055 | 61.764 | 1.00 | 22.63  |
| ATOM | 3150 | O   | GLU | A | 401 | 30.664 | 22.034 | 60.872 | 1.00 | 21.35  |
| ATOM | 3151 | CB  | GLU | A | 401 | 33.915 | 22.247 | 61.648 | 1.00 | 35.39  |
| ATOM | 3152 | CG  | GLU | A | 401 | 35.125 | 23.160 | 61.445 | 1.00 | 70.34  |
| ATOM | 3153 | CD  | GLU | A | 401 | 35.978 | 22.574 | 60.355 | 1.00 | 100.00 |
| ATOM | 3154 | OE1 | GLU | A | 401 | 35.711 | 21.486 | 59.851 | 1.00 | 100.00 |
| ATOM | 3155 | OE2 | GLU | A | 401 | 37.013 | 23.329 | 60.026 | 1.00 | 100.00 |
| ATOM | 3156 | N   | ILE | A | 402 | 31.484 | 21.185 | 62.731 | 1.00 | 20.44  |
| ATOM | 3157 | CA  | ILE | A | 402 | 30.481 | 20.165 | 62.766 | 1.00 | 21.27  |
| ATOM | 3158 | C   | ILE | A | 402 | 29.082 | 20.761 | 62.895 | 1.00 | 26.84  |
| ATOM | 3159 | O   | ILE | A | 402 | 28.142 | 20.366 | 62.199 | 1.00 | 18.68  |
| ATOM | 3160 | CB  | ILE | A | 402 | 30.819 | 19.218 | 63.904 | 1.00 | 24.03  |
| ATOM | 3161 | CG1 | ILE | A | 402 | 31.974 | 18.299 | 63.503 | 1.00 | 23.45  |
| ATOM | 3162 | CG2 | ILE | A | 402 | 29.587 | 18.421 | 64.334 | 1.00 | 28.69  |



60423410-022609

|      |      |     |     |   |     |        |        |        |      |        |
|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
| ATOM | 3224 | CB  | TYR | A | 410 | 18.973 | 22.980 | 59.910 | 1.00 | 19.89  |
| ATOM | 3225 | CG  | TYR | A | 410 | 17.947 | 23.924 | 60.516 | 1.00 | 20.57  |
| ATOM | 3226 | CD1 | TYR | A | 410 | 16.715 | 23.463 | 60.981 | 1.00 | 22.20  |
| ATOM | 3227 | CD2 | TYR | A | 410 | 18.219 | 25.286 | 60.649 | 1.00 | 21.16  |
| ATOM | 3228 | CE1 | TYR | A | 410 | 15.767 | 24.320 | 61.551 | 1.00 | 17.85  |
| ATOM | 3229 | CE2 | TYR | A | 410 | 17.289 | 26.163 | 61.213 | 1.00 | 22.58  |
| ATOM | 3230 | CZ  | TYR | A | 410 | 16.064 | 25.679 | 61.682 | 1.00 | 25.33  |
| ATOM | 3231 | OH  | TYR | A | 410 | 15.182 | 26.528 | 62.315 | 1.00 | 20.84  |
| ATOM | 3232 | N   | VAL | A | 411 | 18.809 | 24.459 | 57.147 | 1.00 | 17.01  |
| ATOM | 3233 | CA  | VAL | A | 411 | 18.378 | 25.520 | 56.254 | 1.00 | 20.36  |
| ATOM | 3234 | C   | VAL | A | 411 | 17.876 | 24.946 | 54.936 | 1.00 | 25.04  |
| ATOM | 3235 | O   | VAL | A | 411 | 16.859 | 25.377 | 54.394 | 1.00 | 22.50  |
| ATOM | 3236 | CB  | VAL | A | 411 | 19.533 | 26.493 | 55.937 | 1.00 | 24.82  |
| ATOM | 3237 | CG1 | VAL | A | 411 | 19.220 | 27.380 | 54.724 | 1.00 | 21.10  |
| ATOM | 3238 | CG2 | VAL | A | 411 | 19.920 | 27.333 | 57.163 | 1.00 | 25.82  |
| ATOM | 3239 | N   | GLU | A | 412 | 18.616 | 23.952 | 54.443 | 1.00 | 24.87  |
| ATOM | 3240 | CA  | GLU | A | 412 | 18.264 | 23.283 | 53.202 | 1.00 | 24.91  |
| ATOM | 3241 | C   | GLU | A | 412 | 16.960 | 22.532 | 53.366 | 1.00 | 24.56  |
| ATOM | 3242 | O   | GLU | A | 412 | 16.045 | 22.612 | 52.555 | 1.00 | 26.86  |
| ATOM | 3243 | CB  | GLU | A | 412 | 19.330 | 22.211 | 52.913 | 1.00 | 28.91  |
| ATOM | 3244 | CG  | GLU | A | 412 | 20.206 | 22.405 | 51.660 | 1.00 | 51.34  |
| ATOM | 3245 | CD  | GLU | A | 412 | 21.671 | 22.089 | 51.908 | 1.00 | 100.00 |
| ATOM | 3246 | OE1 | GLU | A | 412 | 22.243 | 22.331 | 52.963 | 1.00 | 100.00 |
| ATOM | 3247 | OE2 | GLU | A | 412 | 22.274 | 21.541 | 50.874 | 1.00 | 100.00 |
| ATOM | 3248 | N   | LYS | A | 413 | 16.909 | 21.757 | 54.442 | 1.00 | 19.78  |
| ATOM | 3249 | CA  | LYS | A | 413 | 15.755 | 20.940 | 54.747 | 1.00 | 15.53  |
| ATOM | 3250 | C   | LYS | A | 413 | 14.484 | 21.718 | 54.892 | 1.00 | 22.00  |
| ATOM | 3251 | O   | LYS | A | 413 | 13.464 | 21.272 | 54.409 | 1.00 | 23.41  |
| ATOM | 3252 | CB  | LYS | A | 413 | 16.020 | 20.156 | 56.008 | 1.00 | 17.04  |
| ATOM | 3253 | CG  | LYS | A | 413 | 14.754 | 19.602 | 56.629 | 1.00 | 26.97  |
| ATOM | 3254 | CD  | LYS | A | 413 | 14.225 | 18.351 | 55.955 | 1.00 | 37.17  |
| ATOM | 3255 | CE  | LYS | A | 413 | 13.553 | 17.352 | 56.893 | 1.00 | 56.50  |
| ATOM | 3256 | NZ  | LYS | A | 413 | 13.126 | 16.109 | 56.223 | 1.00 | 80.78  |
| ATOM | 3257 | N   | PHE | A | 414 | 14.543 | 22.888 | 55.532 | 1.00 | 19.76  |
| ATOM | 3258 | CA  | PHE | A | 414 | 13.366 | 23.700 | 55.808 | 1.00 | 17.00  |
| ATOM | 3259 | C   | PHE | A | 414 | 13.192 | 24.945 | 54.985 | 1.00 | 21.55  |
| ATOM | 3260 | O   | PHE | A | 414 | 12.329 | 25.748 | 55.303 | 1.00 | 17.11  |
| ATOM | 3261 | CB  | PHE | A | 414 | 13.219 | 24.035 | 57.303 | 1.00 | 16.42  |
| ATOM | 3262 | CG  | PHE | A | 414 | 13.047 | 22.800 | 58.122 | 1.00 | 15.55  |
| ATOM | 3263 | CD1 | PHE | A | 414 | 11.894 | 22.029 | 57.979 | 1.00 | 19.53  |
| ATOM | 3264 | CD2 | PHE | A | 414 | 14.024 | 22.368 | 59.015 | 1.00 | 20.06  |
| ATOM | 3265 | CE1 | PHE | A | 414 | 11.709 | 20.868 | 58.729 | 1.00 | 18.22  |
| ATOM | 3266 | CE2 | PHE | A | 414 | 13.861 | 21.205 | 59.771 | 1.00 | 21.10  |
| ATOM | 3267 | CZ  | PHE | A | 414 | 12.695 | 20.456 | 59.627 | 1.00 | 19.80  |
| ATOM | 3268 | N   | SER | A | 415 | 13.972 | 25.111 | 53.928 | 1.00 | 22.05  |
| ATOM | 3269 | CA  | SER | A | 415 | 13.807 | 26.273 | 53.044 | 1.00 | 23.12  |
| ATOM | 3270 | C   | SER | A | 415 | 12.380 | 26.434 | 52.548 | 1.00 | 23.50  |
| ATOM | 3271 | O   | SER | A | 415 | 11.775 | 25.451 | 52.138 | 1.00 | 22.71  |
| ATOM | 3272 | CB  | SER | A | 415 | 14.763 | 26.214 | 51.858 | 1.00 | 23.04  |
| ATOM | 3273 | OG  | SER | A | 415 | 16.054 | 26.591 | 52.319 | 1.00 | 31.15  |
| ATOM | 3274 | N   | TYR | A | 416 | 11.860 | 27.670 | 52.600 | 1.00 | 21.68  |
| ATOM | 3275 | CA  | TYR | A | 416 | 10.506 | 28.036 | 52.165 | 1.00 | 22.03  |
| ATOM | 3276 | C   | TYR | A | 416 | 9.401  | 27.514 | 53.056 | 1.00 | 22.90  |
| ATOM | 3277 | O   | TYR | A | 416 | 8.239  | 27.556 | 52.681 | 1.00 | 19.44  |
| ATOM | 3278 | CB  | TYR | A | 416 | 10.181 | 27.732 | 50.669 | 1.00 | 21.41  |
| ATOM | 3279 | CG  | TYR | A | 416 | 11.390 | 28.011 | 49.812 | 1.00 | 21.01  |
| ATOM | 3280 | CD1 | TYR | A | 416 | 12.232 | 27.003 | 49.339 | 1.00 | 22.57  |
| ATOM | 3281 | CD2 | TYR | A | 416 | 11.686 | 29.339 | 49.509 | 1.00 | 20.93  |
| ATOM | 3282 | CE1 | TYR | A | 416 | 13.354 | 27.305 | 48.566 | 1.00 | 19.33  |
| ATOM | 3283 | CE2 | TYR | A | 416 | 12.792 | 29.665 | 48.729 | 1.00 | 23.16  |
| ATOM | 3284 | CZ  | TYR | A | 416 | 13.628 | 28.643 | 48.271 | 1.00 | 32.30  |



|      |      |     |     |   |     |        |        |        |      |        |
|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
| ATOM | 3285 | OH  | TYR | A | 416 | 14.715 | 28.959 | 47.491 | 1.00 | 25.33  |
| ATOM | 3286 | N   | LYS | A | 417 | 9.747  | 27.012 | 54.230 | 1.00 | 21.98  |
| ATOM | 3287 | CA  | LYS | A | 417 | 8.749  | 26.482 | 55.127 | 1.00 | 20.82  |
| ATOM | 3288 | C   | LYS | A | 417 | 8.702  | 27.284 | 56.408 | 1.00 | 20.61  |
| ATOM | 3289 | O   | LYS | A | 417 | 9.629  | 28.038 | 56.671 | 1.00 | 18.79  |
| ATOM | 3290 | CB  | LYS | A | 417 | 9.115  | 25.041 | 55.481 | 1.00 | 22.26  |
| ATOM | 3291 | CG  | LYS | A | 417 | 9.094  | 24.078 | 54.266 | 1.00 | 29.52  |
| ATOM | 3292 | CD  | LYS | A | 417 | 7.999  | 24.355 | 53.237 | 1.00 | 72.37  |
| ATOM | 3293 | CE  | LYS | A | 417 | 8.204  | 23.679 | 51.876 | 1.00 | 100.00 |
| ATOM | 3294 | NZ  | LYS | A | 417 | 7.124  | 23.931 | 50.895 | 1.00 | 100.00 |
| ATOM | 3295 | N   | SER | A | 418 | 7.645  | 27.068 | 57.177 | 1.00 | 17.88  |
| ATOM | 3296 | CA  | SER | A | 418 | 7.429  | 27.702 | 58.478 | 1.00 | 19.91  |
| ATOM | 3297 | C   | SER | A | 418 | 7.410  | 26.538 | 59.459 | 1.00 | 23.93  |
| ATOM | 3298 | O   | SER | A | 418 | 6.660  | 25.601 | 59.227 | 1.00 | 21.09  |
| ATOM | 3299 | CB  | SER | A | 418 | 6.139  | 28.495 | 58.451 | 1.00 | 12.45  |
| ATOM | 3300 | OG  | SER | A | 418 | 6.279  | 29.520 | 57.494 | 1.00 | 17.15  |
| ATOM | 3301 | N   | ILE | A | 419 | 8.240  | 26.529 | 60.516 | 1.00 | 14.38  |
| ATOM | 3302 | CA  | ILE | A | 419 | 8.323  | 25.353 | 61.382 | 1.00 | 12.23  |
| ATOM | 3303 | C   | ILE | A | 419 | 8.330  | 25.695 | 62.841 | 1.00 | 16.49  |
| ATOM | 3304 | O   | ILE | A | 419 | 8.334  | 26.875 | 63.219 | 1.00 | 14.48  |
| ATOM | 3305 | CB  | ILE | A | 419 | 9.662  | 24.641 | 61.097 | 1.00 | 18.50  |
| ATOM | 3306 | CG1 | ILE | A | 419 | 10.782 | 25.649 | 61.392 | 1.00 | 18.34  |
| ATOM | 3307 | CG2 | ILE | A | 419 | 9.782  | 24.271 | 59.611 | 1.00 | 14.45  |
| ATOM | 3308 | CD1 | ILE | A | 419 | 12.163 | 25.028 | 61.473 | 1.00 | 22.79  |
| ATOM | 3309 | N   | THR | A | 420 | 8.320  | 24.635 | 63.644 | 1.00 | 16.31  |
| ATOM | 3310 | CA  | THR | A | 420 | 8.281  | 24.810 | 65.083 | 1.00 | 14.71  |
| ATOM | 3311 | C   | THR | A | 420 | 9.545  | 24.290 | 65.714 | 1.00 | 16.25  |
| ATOM | 3312 | O   | THR | A | 420 | 10.346 | 23.636 | 65.077 | 1.00 | 17.31  |
| ATOM | 3313 | CB  | THR | A | 420 | 7.118  | 24.004 | 65.697 | 1.00 | 17.59  |
| ATOM | 3314 | OG1 | THR | A | 420 | 7.437  | 22.645 | 65.519 | 1.00 | 17.59  |
| ATOM | 3315 | CG2 | THR | A | 420 | 5.794  | 24.260 | 65.010 | 1.00 | 16.45  |
| ATOM | 3316 | N   | THR | A | 421 | 9.679  | 24.540 | 67.010 | 1.00 | 15.19  |
| ATOM | 3317 | CA  | THR | A | 421 | 10.782 | 24.047 | 67.818 | 1.00 | 15.49  |
| ATOM | 3318 | C   | THR | A | 421 | 10.930 | 22.520 | 67.618 | 1.00 | 21.17  |
| ATOM | 3319 | O   | THR | A | 421 | 12.041 | 22.044 | 67.401 | 1.00 | 18.91  |
| ATOM | 3320 | CB  | THR | A | 421 | 10.564 | 24.437 | 69.309 | 1.00 | 10.87  |
| ATOM | 3321 | OG1 | THR | A | 421 | 10.618 | 25.851 | 69.383 | 1.00 | 15.99  |
| ATOM | 3322 | CG2 | THR | A | 421 | 11.691 | 23.868 | 70.170 | 1.00 | 11.46  |
| ATOM | 3323 | N   | ASP | A | 422 | 9.829  | 21.736 | 67.673 | 1.00 | 18.70  |
| ATOM | 3324 | CA  | ASP | A | 422 | 9.885  | 20.262 | 67.467 | 1.00 | 16.03  |
| ATOM | 3325 | C   | ASP | A | 422 | 10.469 | 19.867 | 66.107 | 1.00 | 16.08  |
| ATOM | 3326 | O   | ASP | A | 422 | 11.273 | 18.932 | 65.958 | 1.00 | 16.68  |
| ATOM | 3327 | CB  | ASP | A | 422 | 8.523  | 19.568 | 67.581 | 1.00 | 16.64  |
| ATOM | 3328 | CG  | ASP | A | 422 | 8.719  | 18.079 | 67.574 | 1.00 | 26.85  |
| ATOM | 3329 | OD1 | ASP | A | 422 | 9.568  | 17.580 | 68.286 | 1.00 | 23.44  |
| ATOM | 3330 | OD2 | ASP | A | 422 | 7.924  | 17.366 | 66.787 | 1.00 | 23.32  |
| ATOM | 3331 | N   | ASP | A | 423 | 10.069 | 20.575 | 65.060 | 1.00 | 17.50  |
| ATOM | 3332 | CA  | ASP | A | 423 | 10.654 | 20.224 | 63.757 | 1.00 | 18.18  |
| ATOM | 3333 | C   | ASP | A | 423 | 12.148 | 20.442 | 63.826 | 1.00 | 17.70  |
| ATOM | 3334 | O   | ASP | A | 423 | 12.922 | 19.645 | 63.316 | 1.00 | 15.95  |
| ATOM | 3335 | CB  | ASP | A | 423 | 10.099 | 21.075 | 62.613 | 1.00 | 17.77  |
| ATOM | 3336 | CG  | ASP | A | 423 | 8.614  | 20.972 | 62.510 | 1.00 | 20.51  |
| ATOM | 3337 | OD1 | ASP | A | 423 | 8.042  | 19.936 | 62.718 | 1.00 | 29.77  |
| ATOM | 3338 | OD2 | ASP | A | 423 | 8.016  | 22.095 | 62.226 | 1.00 | 18.32  |
| ATOM | 3339 | N   | TRP | A | 424 | 12.559 | 21.545 | 64.459 | 1.00 | 12.60  |
| ATOM | 3340 | CA  | TRP | A | 424 | 13.979 | 21.793 | 64.555 | 1.00 | 14.79  |
| ATOM | 3341 | C   | TRP | A | 424 | 14.690 | 20.684 | 65.330 | 1.00 | 19.67  |
| ATOM | 3342 | O   | TRP | A | 424 | 15.731 | 20.154 | 64.939 | 1.00 | 16.84  |
| ATOM | 3343 | CB  | TRP | A | 424 | 14.187 | 23.134 | 65.283 | 1.00 | 14.84  |
| ATOM | 3344 | CG  | TRP | A | 424 | 15.603 | 23.332 | 65.711 | 1.00 | 13.71  |
| ATOM | 3345 | CD1 | TRP | A | 424 | 16.594 | 23.830 | 64.937 | 1.00 | 15.42  |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 3346 | CD2 | TRP | A | 424 | 16.185 | 23.060 | 67.002 | 1.00 | 13.68 |
| ATOM | 3347 | NE1 | TRP | A | 424 | 17.765 | 23.853 | 65.640 | 1.00 | 14.21 |
| ATOM | 3348 | CE2 | TRP | A | 424 | 17.558 | 23.383 | 66.909 | 1.00 | 13.75 |
| ATOM | 3349 | CE3 | TRP | A | 424 | 15.684 | 22.576 | 68.210 | 1.00 | 16.53 |
| ATOM | 3350 | CZ2 | TRP | A | 424 | 18.436 | 23.247 | 67.983 | 1.00 | 13.89 |
| ATOM | 3351 | CZ3 | TRP | A | 424 | 16.564 | 22.434 | 69.288 | 1.00 | 16.24 |
| ATOM | 3352 | CH2 | TRP | A | 424 | 17.919 | 22.786 | 69.175 | 1.00 | 15.55 |
| ATOM | 3353 | N   | LYS | A | 425 | 14.139 | 20.328 | 66.480 | 1.00 | 13.83 |
| ATOM | 3354 | CA  | LYS | A | 425 | 14.778 | 19.337 | 67.319 | 1.00 | 14.35 |
| ATOM | 3355 | C   | LYS | A | 425 | 14.705 | 17.914 | 66.753 | 1.00 | 19.43 |
| ATOM | 3356 | O   | LYS | A | 425 | 15.619 | 17.089 | 66.910 | 1.00 | 16.20 |
| ATOM | 3357 | CB  | LYS | A | 425 | 14.262 | 19.441 | 68.735 | 1.00 | 13.53 |
| ATOM | 3358 | CG  | LYS | A | 425 | 14.912 | 18.488 | 69.720 | 1.00 | 14.17 |
| ATOM | 3359 | CD  | LYS | A | 425 | 14.289 | 18.698 | 71.085 | 1.00 | 14.61 |
| ATOM | 3360 | CE  | LYS | A | 425 | 14.214 | 17.413 | 71.872 | 1.00 | 33.75 |
| ATOM | 3361 | NZ  | LYS | A | 425 | 12.961 | 16.707 | 71.574 | 1.00 | 28.69 |
| ATOM | 3362 | N   | ASP | A | 426 | 13.591 | 17.633 | 66.093 | 1.00 | 17.34 |
| ATOM | 3363 | CA  | ASP | A | 426 | 13.430 | 16.341 | 65.480 | 1.00 | 15.98 |
| ATOM | 3364 | C   | ASP | A | 426 | 14.524 | 16.256 | 64.383 | 1.00 | 23.28 |
| ATOM | 3365 | O   | ASP | A | 426 | 15.177 | 15.246 | 64.128 | 1.00 | 25.50 |
| ATOM | 3366 | CB  | ASP | A | 426 | 11.987 | 16.225 | 64.918 | 1.00 | 13.29 |
| ATOM | 3367 | CG  | ASP | A | 426 | 10.984 | 15.900 | 65.989 | 1.00 | 14.86 |
| ATOM | 3368 | OD1 | ASP | A | 426 | 11.296 | 15.712 | 67.147 | 1.00 | 19.08 |
| ATOM | 3369 | OD2 | ASP | A | 426 | 9.746  | 15.852 | 65.579 | 1.00 | 18.33 |
| ATOM | 3370 | N   | PHE | A | 427 | 14.770 | 17.354 | 63.684 | 1.00 | 20.60 |
| ATOM | 3371 | CA  | PHE | A | 427 | 15.789 | 17.331 | 62.633 | 1.00 | 20.61 |
| ATOM | 3372 | C   | PHE | A | 427 | 17.203 | 17.172 | 63.165 | 1.00 | 26.34 |
| ATOM | 3373 | O   | PHE | A | 427 | 18.056 | 16.476 | 62.592 | 1.00 | 22.98 |
| ATOM | 3374 | CB  | PHE | A | 427 | 15.712 | 18.535 | 61.679 | 1.00 | 20.77 |
| ATOM | 3375 | CG  | PHE | A | 427 | 16.772 | 18.432 | 60.611 | 1.00 | 24.06 |
| ATOM | 3376 | CD1 | PHE | A | 427 | 16.747 | 17.398 | 59.674 | 1.00 | 27.11 |
| ATOM | 3377 | CD2 | PHE | A | 427 | 17.815 | 19.355 | 60.549 | 1.00 | 24.52 |
| ATOM | 3378 | CE1 | PHE | A | 427 | 17.726 | 17.312 | 58.685 | 1.00 | 27.68 |
| ATOM | 3379 | CE2 | PHE | A | 427 | 18.801 | 19.284 | 59.565 | 1.00 | 28.65 |
| ATOM | 3380 | CZ  | PHE | A | 427 | 18.756 | 18.254 | 58.629 | 1.00 | 24.74 |
| ATOM | 3381 | N   | LEU | A | 428 | 17.417 | 17.848 | 64.291 | 1.00 | 22.50 |
| ATOM | 3382 | CA  | LEU | A | 428 | 18.686 | 17.827 | 64.979 | 1.00 | 24.10 |
| ATOM | 3383 | C   | LEU | A | 428 | 19.053 | 16.391 | 65.339 | 1.00 | 22.01 |
| ATOM | 3384 | O   | LEU | A | 428 | 20.183 | 15.960 | 65.123 | 1.00 | 23.99 |
| ATOM | 3385 | CB  | LEU | A | 428 | 18.685 | 18.806 | 66.186 | 1.00 | 23.18 |
| ATOM | 3386 | CG  | LEU | A | 428 | 19.949 | 18.790 | 67.054 | 1.00 | 26.21 |
| ATOM | 3387 | CD1 | LEU | A | 428 | 21.120 | 19.538 | 66.421 | 1.00 | 25.09 |
| ATOM | 3388 | CD2 | LEU | A | 428 | 19.659 | 19.334 | 68.459 | 1.00 | 21.07 |
| ATOM | 3389 | N   | TYR | A | 429 | 18.087 | 15.650 | 65.866 | 1.00 | 16.35 |
| ATOM | 3390 | CA  | TYR | A | 429 | 18.278 | 14.259 | 66.241 | 1.00 | 15.82 |
| ATOM | 3391 | C   | TYR | A | 429 | 18.482 | 13.390 | 65.019 | 1.00 | 20.80 |
| ATOM | 3392 | O   | TYR | A | 429 | 19.216 | 12.416 | 64.997 | 1.00 | 21.02 |
| ATOM | 3393 | CB  | TYR | A | 429 | 17.037 | 13.759 | 66.940 | 1.00 | 14.93 |
| ATOM | 3394 | CG  | TYR | A | 429 | 17.232 | 13.841 | 68.426 | 1.00 | 19.52 |
| ATOM | 3395 | CD1 | TYR | A | 429 | 16.999 | 15.039 | 69.104 | 1.00 | 18.07 |
| ATOM | 3396 | CD2 | TYR | A | 429 | 17.667 | 12.710 | 69.121 | 1.00 | 17.20 |
| ATOM | 3397 | CE1 | TYR | A | 429 | 17.183 | 15.108 | 70.484 | 1.00 | 14.78 |
| ATOM | 3398 | CE2 | TYR | A | 429 | 17.850 | 12.752 | 70.496 | 1.00 | 15.85 |
| ATOM | 3399 | CZ  | TYR | A | 429 | 17.615 | 13.961 | 71.157 | 1.00 | 26.56 |
| ATOM | 3400 | OH  | TYR | A | 429 | 17.807 | 14.009 | 72.508 | 1.00 | 23.93 |
| ATOM | 3401 | N   | SER | A | 430 | 17.839 | 13.785 | 63.955 | 1.00 | 18.00 |
| ATOM | 3402 | CA  | SER | A | 430 | 17.986 | 13.048 | 62.735 | 1.00 | 20.34 |
| ATOM | 3403 | C   | SER | A | 430 | 19.392 | 13.282 | 62.136 | 1.00 | 28.86 |
| ATOM | 3404 | O   | SER | A | 430 | 20.133 | 12.347 | 61.797 | 1.00 | 25.84 |
| ATOM | 3405 | CB  | SER | A | 430 | 16.843 | 13.486 | 61.845 | 1.00 | 19.64 |
| ATOM | 3406 | OG  | SER | A | 430 | 16.960 | 12.766 | 60.657 | 1.00 | 32.88 |



|      |      |     |     |   |     |        |        |        |      |        |
|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
| ATOM | 3407 | N   | TYR | A | 431 | 19.792 | 14.556 | 62.021 | 1.00 | 23.08  |
| ATOM | 3408 | CA  | TYR | A | 431 | 21.104 | 14.862 | 61.497 | 1.00 | 23.26  |
| ATOM | 3409 | C   | TYR | A | 431 | 22.209 | 14.166 | 62.288 | 1.00 | 31.19  |
| ATOM | 3410 | O   | TYR | A | 431 | 23.152 | 13.580 | 61.747 | 1.00 | 27.84  |
| ATOM | 3411 | CB  | TYR | A | 431 | 21.392 | 16.372 | 61.476 | 1.00 | 22.23  |
| ATOM | 3412 | CG  | TYR | A | 431 | 22.660 | 16.758 | 60.741 | 1.00 | 23.21  |
| ATOM | 3413 | CD1 | TYR | A | 431 | 22.665 | 16.994 | 59.365 | 1.00 | 26.21  |
| ATOM | 3414 | CD2 | TYR | A | 431 | 23.864 | 16.920 | 61.433 | 1.00 | 28.30  |
| ATOM | 3415 | CE1 | TYR | A | 431 | 23.836 | 17.354 | 58.692 | 1.00 | 33.33  |
| ATOM | 3416 | CE2 | TYR | A | 431 | 25.045 | 17.277 | 60.777 | 1.00 | 29.03  |
| ATOM | 3417 | CZ  | TYR | A | 431 | 25.032 | 17.498 | 59.401 | 1.00 | 33.73  |
| ATOM | 3418 | OH  | TYR | A | 431 | 26.201 | 17.881 | 58.802 | 1.00 | 30.59  |
| ATOM | 3419 | N   | PHE | A | 432 | 22.078 | 14.272 | 63.608 | 1.00 | 23.42  |
| ATOM | 3420 | CA  | PHE | A | 432 | 23.039 | 13.735 | 64.556 | 1.00 | 22.14  |
| ATOM | 3421 | C   | PHE | A | 432 | 22.659 | 12.334 | 65.001 | 1.00 | 27.48  |
| ATOM | 3422 | O   | PHE | A | 432 | 22.824 | 11.964 | 66.168 | 1.00 | 20.81  |
| ATOM | 3423 | CB  | PHE | A | 432 | 23.211 | 14.715 | 65.751 | 1.00 | 20.76  |
| ATOM | 3424 | CG  | PHE | A | 432 | 24.035 | 15.918 | 65.348 | 1.00 | 21.62  |
| ATOM | 3425 | CD1 | PHE | A | 432 | 25.364 | 15.674 | 65.025 | 1.00 | 25.75  |
| ATOM | 3426 | CD2 | PHE | A | 432 | 23.566 | 17.232 | 65.250 | 1.00 | 22.01  |
| ATOM | 3427 | CE1 | PHE | A | 432 | 26.202 | 16.708 | 64.619 | 1.00 | 26.06  |
| ATOM | 3428 | CE2 | PHE | A | 432 | 24.398 | 18.277 | 64.841 | 1.00 | 24.06  |
| ATOM | 3429 | CZ  | PHE | A | 432 | 25.732 | 18.014 | 64.539 | 1.00 | 22.97  |
| ATOM | 3430 | N   | LYS | A | 433 | 22.150 | 11.536 | 64.065 | 1.00 | 30.29  |
| ATOM | 3431 | CA  | LYS | A | 433 | 21.757 | 10.205 | 64.480 | 1.00 | 33.97  |
| ATOM | 3432 | C   | LYS | A | 433 | 22.886 | 9.408  | 65.113 | 1.00 | 40.77  |
| ATOM | 3433 | O   | LYS | A | 433 | 22.690 | 8.545  | 65.964 | 1.00 | 45.44  |
| ATOM | 3434 | CB  | LYS | A | 433 | 21.017 | 9.429  | 63.418 | 1.00 | 41.36  |
| ATOM | 3435 | CG  | LYS | A | 433 | 21.934 | 9.107  | 62.270 | 1.00 | 42.12  |
| ATOM | 3436 | CD  | LYS | A | 433 | 21.340 | 9.569  | 60.951 | 1.00 | 85.11  |
| ATOM | 3437 | CE  | LYS | A | 433 | 21.770 | 8.690  | 59.784 | 1.00 | 100.00 |
| ATOM | 3438 | NZ  | LYS | A | 433 | 21.052 | 8.990  | 58.530 | 1.00 | 100.00 |
| ATOM | 3439 | N   | ASP | A | 434 | 24.091 | 9.729  | 64.700 | 1.00 | 38.33  |
| ATOM | 3440 | CA  | ASP | A | 434 | 25.295 | 9.086  | 65.188 | 1.00 | 40.98  |
| ATOM | 3441 | C   | ASP | A | 434 | 25.640 | 9.549  | 66.594 | 1.00 | 42.43  |
| ATOM | 3442 | O   | ASP | A | 434 | 26.508 | 8.979  | 67.241 | 1.00 | 42.35  |
| ATOM | 3443 | CB  | ASP | A | 434 | 26.493 | 9.429  | 64.250 | 1.00 | 47.81  |
| ATOM | 3444 | CG  | ASP | A | 434 | 26.762 | 10.919 | 64.034 | 1.00 | 73.28  |
| ATOM | 3445 | OD1 | ASP | A | 434 | 25.948 | 11.739 | 63.601 | 1.00 | 69.11  |
| ATOM | 3446 | OD2 | ASP | A | 434 | 28.007 | 11.242 | 64.314 | 1.00 | 80.38  |
| ATOM | 3447 | N   | LYS | A | 435 | 24.987 | 10.601 | 67.068 | 1.00 | 33.72  |
| ATOM | 3448 | CA  | LYS | A | 435 | 25.312 | 11.120 | 68.374 | 1.00 | 30.49  |
| ATOM | 3449 | C   | LYS | A | 435 | 24.122 |        |        |      |        |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 3468 | CG  | ASP | A | 437 | 23.976 | 7.123  | 73.303 | 1.00 | 64.05 |
| ATOM | 3469 | OD1 | ASP | A | 437 | 22.749 | 7.018  | 73.361 | 1.00 | 57.77 |
| ATOM | 3470 | OD2 | ASP | A | 437 | 24.825 | 6.121  | 73.385 | 1.00 | 89.95 |
| ATOM | 3471 | N   | VAL | A | 438 | 24.778 | 11.697 | 72.826 | 1.00 | 33.10 |
| ATOM | 3472 | CA  | VAL | A | 438 | 25.235 | 12.988 | 73.309 | 1.00 | 31.59 |
| ATOM | 3473 | C   | VAL | A | 438 | 24.012 | 13.879 | 73.521 | 1.00 | 28.65 |
| ATOM | 3474 | O   | VAL | A | 438 | 23.828 | 14.461 | 74.571 | 1.00 | 26.75 |
| ATOM | 3475 | CB  | VAL | A | 438 | 26.289 | 13.599 | 72.371 | 1.00 | 30.58 |
| ATOM | 3476 | CG1 | VAL | A | 438 | 26.809 | 14.928 | 72.920 | 1.00 | 27.87 |
| ATOM | 3477 | CG2 | VAL | A | 438 | 27.441 | 12.608 | 72.226 | 1.00 | 29.01 |
| ATOM | 3478 | N   | LEU | A | 439 | 23.179 | 13.926 | 72.494 | 1.00 | 22.69 |
| ATOM | 3479 | CA  | LEU | A | 439 | 21.952 | 14.698 | 72.466 | 1.00 | 20.02 |
| ATOM | 3480 | C   | LEU | A | 439 | 21.118 | 14.396 | 73.675 | 1.00 | 28.06 |
| ATOM | 3481 | O   | LEU | A | 439 | 20.547 | 15.279 | 74.289 | 1.00 | 31.30 |
| ATOM | 3482 | CB  | LEU | A | 439 | 21.125 | 14.403 | 71.201 | 1.00 | 17.24 |
| ATOM | 3483 | CG  | LEU | A | 439 | 21.769 | 15.002 | 69.960 | 1.00 | 19.41 |
| ATOM | 3484 | CD1 | LEU | A | 439 | 21.029 | 14.542 | 68.724 | 1.00 | 16.82 |
| ATOM | 3485 | CD2 | LEU | A | 439 | 21.748 | 16.528 | 70.034 | 1.00 | 23.96 |
| ATOM | 3486 | N   | ASN | A | 440 | 21.045 | 13.129 | 74.022 | 1.00 | 24.23 |
| ATOM | 3487 | CA  | ASN | A | 440 | 20.242 | 12.765 | 75.165 | 1.00 | 24.80 |
| ATOM | 3488 | C   | ASN | A | 440 | 20.785 | 13.294 | 76.473 | 1.00 | 29.26 |
| ATOM | 3489 | O   | ASN | A | 440 | 20.128 | 13.233 | 77.507 | 1.00 | 31.02 |
| ATOM | 3490 | CB  | ASN | A | 440 | 19.842 | 11.275 | 75.237 | 1.00 | 28.06 |
| ATOM | 3491 | CG  | ASN | A | 440 | 18.971 | 10.884 | 74.066 | 1.00 | 29.31 |
| ATOM | 3492 | OD1 | ASN | A | 440 | 19.138 | 9.820  | 73.451 | 1.00 | 40.12 |
| ATOM | 3493 | ND2 | ASN | A | 440 | 18.058 | 11.773 | 73.721 | 1.00 | 28.40 |
| ATOM | 3494 | N   | GLN | A | 441 | 21.984 | 13.833 | 76.434 | 1.00 | 26.30 |
| ATOM | 3495 | CA  | GLN | A | 441 | 22.535 | 14.361 | 77.656 | 1.00 | 27.26 |
| ATOM | 3496 | C   | GLN | A | 441 | 22.022 | 15.764 | 77.912 | 1.00 | 26.46 |
| ATOM | 3497 | O   | GLN | A | 441 | 22.203 | 16.336 | 78.988 | 1.00 | 25.27 |
| ATOM | 3498 | CB  | GLN | A | 441 | 24.073 | 14.404 | 77.609 | 1.00 | 32.14 |
| ATOM | 3499 | CG  | GLN | A | 441 | 24.762 | 13.016 | 77.641 | 1.00 | 49.60 |
| ATOM | 3500 | CD  | GLN | A | 441 | 26.057 | 13.019 | 76.850 | 1.00 | 66.63 |
| ATOM | 3501 | OE1 | GLN | A | 441 | 26.546 | 11.975 | 76.382 | 1.00 | 76.27 |
| ATOM | 3502 | NE2 | GLN | A | 441 | 26.608 | 14.217 | 76.676 | 1.00 | 56.68 |
| ATOM | 3503 | N   | VAL | A | 442 | 21.388 | 16.345 | 76.909 | 1.00 | 21.59 |
| ATOM | 3504 | CA  | VAL | A | 442 | 20.922 | 17.688 | 77.159 | 1.00 | 18.91 |
| ATOM | 3505 | C   | VAL | A | 442 | 19.615 | 17.729 | 77.897 | 1.00 | 19.52 |
| ATOM | 3506 | O   | VAL | A | 442 | 18.742 | 16.908 | 77.650 | 1.00 | 21.02 |
| ATOM | 3507 | CB  | VAL | A | 442 | 20.898 | 18.538 | 75.917 | 1.00 | 19.77 |
| ATOM | 3508 | CG1 | VAL | A | 442 | 21.472 | 17.891 | 74.680 | 1.00 | 23.00 |
| ATOM | 3509 | CG2 | VAL | A | 442 | 19.787 | 19.580 | 75.787 | 1.00 | 13.26 |
| ATOM | 3510 | N   | ASP | A | 443 | 19.490 | 18.677 | 78.811 | 1.00 | 17.20 |
| ATOM | 3511 | CA  | ASP | A | 443 | 18.243 | 18.856 | 79.551 | 1.00 | 16.44 |
| ATOM | 3512 | C   | ASP | A | 443 | 17.277 | 19.752 | 78.727 | 1.00 | 17.64 |
| ATOM | 3513 | O   | ASP | A | 443 | 17.091 | 20.980 | 78.921 | 1.00 | 15.06 |
| ATOM | 3514 | CB  | ASP | A | 443 | 18.611 | 19.494 | 80.901 | 1.00 | 17.40 |
| ATOM | 3515 | CG  | ASP | A | 443 | 17.422 | 19.595 | 81.778 | 1.00 | 21.50 |
| ATOM | 3516 | OD1 | ASP | A | 443 | 16.309 | 19.286 | 81.395 | 1.00 | 26.57 |
| ATOM | 3517 | OD2 | ASP | A | 443 | 17.731 | 20.068 | 82.959 | 1.00 | 23.49 |
| ATOM | 3518 | N   | TRP | A | 444 | 16.675 | 19.105 | 77.736 | 1.00 | 15.54 |
| ATOM | 3519 | CA  | TRP | A | 444 | 15.763 | 19.759 | 76.816 | 1.00 | 16.92 |
| ATOM | 3520 | C   | TRP | A | 444 | 14.641 | 20.468 | 77.546 | 1.00 | 19.29 |
| ATOM | 3521 | O   | TRP | A | 444 | 14.292 | 21.572 | 77.194 | 1.00 | 18.00 |
| ATOM | 3522 | CB  | TRP | A | 444 | 15.195 | 18.747 | 75.793 | 1.00 | 13.71 |
| ATOM | 3523 | CG  | TRP | A | 444 | 16.267 | 18.226 | 74.892 | 1.00 | 14.88 |
| ATOM | 3524 | CD1 | TRP | A | 444 | 16.797 | 16.969 | 74.872 | 1.00 | 17.32 |
| ATOM | 3525 | CD2 | TRP | A | 444 | 16.952 | 18.958 | 73.861 | 1.00 | 16.34 |
| ATOM | 3526 | NE1 | TRP | A | 444 | 17.779 | 16.869 | 73.915 | 1.00 | 14.83 |
| ATOM | 3527 | CE2 | TRP | A | 444 | 17.880 | 18.063 | 73.255 | 1.00 | 16.96 |
| ATOM | 3528 | CE3 | TRP | A | 444 | 16.896 | 20.295 | 73.415 | 1.00 | 17.06 |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 3529 | CZ2 | TRP | A | 444 | 18.737 | 18.482 | 72.229 | 1.00 | 16.95 |
| ATOM | 3530 | CZ3 | TRP | A | 444 | 17.750 | 20.697 | 72.382 | 1.00 | 16.35 |
| ATOM | 3531 | CH2 | TRP | A | 444 | 18.664 | 19.807 | 71.806 | 1.00 | 16.47 |
| ATOM | 3532 | N   | ASN | A | 445 | 14.059 | 19.808 | 78.557 | 1.00 | 18.46 |
| ATOM | 3533 | CA  | ASN | A | 445 | 12.957 | 20.414 | 79.260 | 1.00 | 17.22 |
| ATOM | 3534 | C   | ASN | A | 445 | 13.334 | 21.761 | 79.837 | 1.00 | 20.45 |
| ATOM | 3535 | O   | ASN | A | 445 | 12.581 | 22.732 | 79.740 | 1.00 | 17.51 |
| ATOM | 3536 | CB  | ASN | A | 445 | 12.347 | 19.512 | 80.357 | 1.00 | 15.11 |
| ATOM | 3537 | CG  | ASN | A | 445 | 11.322 | 20.272 | 81.234 | 1.00 | 46.40 |
| ATOM | 3538 | OD1 | ASN | A | 445 | 11.526 | 20.515 | 82.448 | 1.00 | 39.99 |
| ATOM | 3539 | ND2 | ASN | A | 445 | 10.198 | 20.671 | 80.643 | 1.00 | 26.34 |
| ATOM | 3540 | N   | ALA | A | 446 | 14.504 | 21.791 | 80.484 | 1.00 | 18.70 |
| ATOM | 3541 | CA  | ALA | A | 446 | 14.918 | 23.022 | 81.091 | 1.00 | 16.75 |
| ATOM | 3542 | C   | ALA | A | 446 | 15.272 | 24.029 | 80.032 | 1.00 | 21.46 |
| ATOM | 3543 | O   | ALA | A | 446 | 14.765 | 25.172 | 80.030 | 1.00 | 20.55 |
| ATOM | 3544 | CB  | ALA | A | 446 | 16.049 | 22.774 | 82.055 | 1.00 | 19.42 |
| ATOM | 3545 | N   | TRP | A | 447 | 16.116 | 23.605 | 79.097 | 1.00 | 16.36 |
| ATOM | 3546 | CA  | TRP | A | 447 | 16.476 | 24.563 | 78.054 | 1.00 | 14.85 |
| ATOM | 3547 | C   | TRP | A | 447 | 15.277 | 25.163 | 77.279 | 1.00 | 18.68 |
| ATOM | 3548 | O   | TRP | A | 447 | 15.246 | 26.365 | 76.985 | 1.00 | 14.03 |
| ATOM | 3549 | CB  | TRP | A | 447 | 17.473 | 23.938 | 77.040 | 1.00 | 17.25 |
| ATOM | 3550 | CG  | TRP | A | 447 | 18.952 | 23.982 | 77.391 | 1.00 | 19.35 |
| ATOM | 3551 | CD1 | TRP | A | 447 | 19.697 | 22.957 | 77.930 | 1.00 | 22.25 |
| ATOM | 3552 | CD2 | TRP | A | 447 | 19.864 | 25.090 | 77.224 | 1.00 | 16.70 |
| ATOM | 3553 | NE1 | TRP | A | 447 | 21.007 | 23.356 | 78.105 | 1.00 | 19.46 |
| ATOM | 3554 | CE2 | TRP | A | 447 | 21.131 | 24.662 | 77.679 | 1.00 | 18.42 |
| ATOM | 3555 | CE3 | TRP | A | 447 | 19.737 | 26.403 | 76.766 | 1.00 | 16.34 |
| ATOM | 3556 | CZ2 | TRP | A | 447 | 22.241 | 25.512 | 77.625 | 1.00 | 16.76 |
| ATOM | 3557 | CZ3 | TRP | A | 447 | 20.854 | 27.230 | 76.705 | 1.00 | 14.87 |
| ATOM | 3558 | CH2 | TRP | A | 447 | 22.090 | 26.786 | 77.141 | 1.00 | 14.22 |
| ATOM | 3559 | N   | LEU | A | 448 | 14.275 | 24.336 | 76.899 | 1.00 | 14.96 |
| ATOM | 3560 | CA  | LEU | A | 448 | 13.146 | 24.835 | 76.096 | 1.00 | 16.27 |
| ATOM | 3561 | C   | LEU | A | 448 | 11.995 | 25.464 | 76.877 | 1.00 | 17.91 |
| ATOM | 3562 | O   | LEU | A | 448 | 11.332 | 26.404 | 76.398 | 1.00 | 13.49 |
| ATOM | 3563 | CB  | LEU | A | 448 | 12.522 | 23.690 | 75.238 | 1.00 | 16.42 |
| ATOM | 3564 | CG  | LEU | A | 448 | 13.500 | 22.945 | 74.302 | 1.00 | 16.43 |
| ATOM | 3565 | CD1 | LEU | A | 448 | 12.845 | 21.795 | 73.536 | 1.00 | 15.65 |
| ATOM | 3566 | CD2 | LEU | A | 448 | 14.163 | 23.901 | 73.315 | 1.00 | 12.87 |
| ATOM | 3567 | N   | TYR | A | 449 | 11.733 | 24.874 | 78.048 | 1.00 | 15.32 |
| ATOM | 3568 | CA  | TYR | A | 449 | 10.557 | 25.255 | 78.826 | 1.00 | 15.36 |
| ATOM | 3569 | C   | TYR | A | 449 | 10.763 | 25.822 | 80.198 | 1.00 | 19.93 |
| ATOM | 3570 | O   | TYR | A | 449 | 9.763  | 26.226 | 80.806 | 1.00 | 21.29 |
| ATOM | 3571 | CB  | TYR | A |     |        |        |        |      |       |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 3590 | CG  | PRO | A | 451 | 10.903 | 29.560 | 84.988 | 1.00 | 16.01 |
| ATOM | 3591 | CD  | PRO | A | 451 | 11.298 | 28.259 | 84.288 | 1.00 | 15.25 |
| ATOM | 3592 | N   | GLY | A | 452 | 14.148 | 31.481 | 83.586 | 1.00 | 12.85 |
| ATOM | 3593 | CA  | GLY | A | 452 | 15.430 | 31.822 | 84.160 | 1.00 | 12.46 |
| ATOM | 3594 | C   | GLY | A | 452 | 16.652 | 31.517 | 83.311 | 1.00 | 17.53 |
| ATOM | 3595 | O   | GLY | A | 452 | 16.559 | 31.320 | 82.117 | 1.00 | 14.38 |
| ATOM | 3596 | N   | LEU | A | 453 | 17.839 | 31.539 | 83.926 | 1.00 | 17.18 |
| ATOM | 3597 | CA  | LEU | A | 453 | 19.054 | 31.268 | 83.196 | 1.00 | 14.53 |
| ATOM | 3598 | C   | LEU | A | 453 | 19.087 | 29.819 | 82.762 | 1.00 | 14.71 |
| ATOM | 3599 | O   | LEU | A | 453 | 18.523 | 28.978 | 83.456 | 1.00 | 16.06 |
| ATOM | 3600 | CB  | LEU | A | 453 | 20.296 | 31.588 | 84.031 | 1.00 | 14.09 |
| ATOM | 3601 | CG  | LEU | A | 453 | 20.526 | 33.091 | 84.216 | 1.00 | 18.81 |
| ATOM | 3602 | CD1 | LEU | A | 453 | 21.635 | 33.253 | 85.247 | 1.00 | 16.98 |
| ATOM | 3603 | CD2 | LEU | A | 453 | 21.001 | 33.761 | 82.919 | 1.00 | 21.45 |
| ATOM | 3604 | N   | PRO | A | 454 | 19.770 | 29.537 | 81.637 | 1.00 | 15.62 |
| ATOM | 3605 | CA  | PRO | A | 454 | 19.907 | 28.194 | 81.119 | 1.00 | 15.68 |
| ATOM | 3606 | C   | PRO | A | 454 | 20.486 | 27.258 | 82.170 | 1.00 | 21.35 |
| ATOM | 3607 | O   | PRO | A | 454 | 21.236 | 27.662 | 83.039 | 1.00 | 21.73 |
| ATOM | 3608 | CB  | PRO | A | 454 | 20.918 | 28.317 | 79.965 | 1.00 | 16.56 |
| ATOM | 3609 | CG  | PRO | A | 454 | 20.906 | 29.751 | 79.501 | 1.00 | 16.74 |
| ATOM | 3610 | CD  | PRO | A | 454 | 20.290 | 30.524 | 80.640 | 1.00 | 15.71 |
| ATOM | 3611 | N   | PRO | A | 455 | 20.146 | 25.978 | 82.079 | 1.00 | 16.53 |
| ATOM | 3612 | CA  | PRO | A | 455 | 20.619 | 24.976 | 83.005 | 1.00 | 16.33 |
| ATOM | 3613 | C   | PRO | A | 455 | 22.146 | 24.834 | 83.016 | 1.00 | 25.51 |
| ATOM | 3614 | O   | PRO | A | 455 | 22.718 | 24.370 | 83.999 | 1.00 | 24.17 |
| ATOM | 3615 | CB  | PRO | A | 455 | 19.999 | 23.666 | 82.520 | 1.00 | 17.40 |
| ATOM | 3616 | CG  | PRO | A | 455 | 19.523 | 23.888 | 81.094 | 1.00 | 21.81 |
| ATOM | 3617 | CD  | PRO | A | 455 | 19.403 | 25.389 | 80.932 | 1.00 | 19.90 |
| ATOM | 3618 | N   | ILE | A | 456 | 22.816 | 25.205 | 81.916 | 1.00 | 20.88 |
| ATOM | 3619 | CA  | ILE | A | 456 | 24.262 | 25.117 | 81.810 | 1.00 | 17.40 |
| ATOM | 3620 | C   | ILE | A | 456 | 24.822 | 26.292 | 81.000 | 1.00 | 19.27 |
| ATOM | 3621 | O   | ILE | A | 456 | 24.191 | 26.798 | 80.064 | 1.00 | 17.96 |
| ATOM | 3622 | CB  | ILE | A | 456 | 24.675 | 23.737 | 81.316 | 1.00 | 23.45 |
| ATOM | 3623 | CG1 | ILE | A | 456 | 26.173 | 23.543 | 81.456 | 1.00 | 27.66 |
| ATOM | 3624 | CG2 | ILE | A | 456 | 24.285 | 23.529 | 79.865 | 1.00 | 26.37 |
| ATOM | 3625 | CD1 | ILE | A | 456 | 26.571 | 22.167 | 80.951 | 1.00 | 35.97 |
| ATOM | 3626 | N   | LYS | A | 457 | 26.011 | 26.772 | 81.383 | 1.00 | 15.81 |
| ATOM | 3627 | CA  | LYS | A | 457 | 26.649 | 27.883 | 80.697 | 1.00 | 17.12 |
| ATOM | 3628 | C   | LYS | A | 457 | 27.727 | 27.333 | 79.815 | 1.00 | 18.91 |
| ATOM | 3629 | O   | LYS | A | 457 | 28.541 | 26.562 | 80.281 | 1.00 | 17.84 |
| ATOM | 3630 | CB  | LYS | A | 457 | 27.308 | 28.793 | 81.727 | 1.00 | 16.24 |
| ATOM | 3631 | CG  | LYS | A | 457 | 27.896 | 30.067 | 81.130 | 1.00 | 16.93 |
| ATOM | 3632 | CD  | LYS | A | 457 | 28.245 | 3      |        |      |       |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 3651 | CA  | TYR | A | 460 | 34.021 | 30.994 | 76.536 | 1.00 | 14.52 |
| ATOM | 3652 | C   | TYR | A | 460 | 35.485 | 31.370 | 76.683 | 1.00 | 16.97 |
| ATOM | 3653 | O   | TYR | A | 460 | 36.003 | 31.442 | 77.802 | 1.00 | 13.34 |
| ATOM | 3654 | CB  | TYR | A | 460 | 33.266 | 32.254 | 76.990 | 1.00 | 12.53 |
| ATOM | 3655 | CG  | TYR | A | 460 | 31.764 | 32.129 | 76.980 | 1.00 | 13.07 |
| ATOM | 3656 | CD1 | TYR | A | 460 | 31.070 | 31.553 | 78.046 | 1.00 | 17.79 |
| ATOM | 3657 | CD2 | TYR | A | 460 | 31.043 | 32.584 | 75.880 | 1.00 | 12.08 |
| ATOM | 3658 | CE1 | TYR | A | 460 | 29.677 | 31.450 | 78.049 | 1.00 | 16.54 |
| ATOM | 3659 | CE2 | TYR | A | 460 | 29.654 | 32.477 | 75.861 | 1.00 | 11.82 |
| ATOM | 3660 | CZ  | TYR | A | 460 | 28.971 | 31.911 | 76.938 | 1.00 | 16.71 |
| ATOM | 3661 | OH  | TYR | A | 460 | 27.589 | 31.834 | 76.894 | 1.00 | 15.52 |
| ATOM | 3662 | N   | ASP | A | 461 | 36.098 | 31.706 | 75.558 | 1.00 | 13.99 |
| ATOM | 3663 | CA  | ASP | A | 461 | 37.463 | 32.218 | 75.579 | 1.00 | 13.74 |
| ATOM | 3664 | C   | ASP | A | 461 | 37.414 | 33.608 | 76.255 | 1.00 | 16.51 |
| ATOM | 3665 | O   | ASP | A | 461 | 36.516 | 34.415 | 75.966 | 1.00 | 15.04 |
| ATOM | 3666 | CB  | ASP | A | 461 | 37.968 | 32.336 | 74.133 | 1.00 | 12.98 |
| ATOM | 3667 | CG  | ASP | A | 461 | 39.393 | 32.801 | 74.148 | 1.00 | 25.31 |
| ATOM | 3668 | OD1 | ASP | A | 461 | 40.335 | 32.064 | 74.314 | 1.00 | 40.40 |
| ATOM | 3669 | OD2 | ASP | A | 461 | 39.520 | 34.087 | 74.051 | 1.00 | 19.41 |
| ATOM | 3670 | N   | MET | A | 462 | 38.339 | 33.887 | 77.191 | 1.00 | 12.14 |
| ATOM | 3671 | CA  | MET | A | 462 | 38.359 | 35.144 | 77.928 | 1.00 | 9.92  |
| ATOM | 3672 | C   | MET | A | 462 | 39.312 | 36.203 | 77.406 | 1.00 | 15.43 |
| ATOM | 3673 | O   | MET | A | 462 | 39.413 | 37.265 | 77.958 | 1.00 | 15.61 |
| ATOM | 3674 | CB  | MET | A | 462 | 38.688 | 34.910 | 79.404 | 1.00 | 9.27  |
| ATOM | 3675 | CG  | MET | A | 462 | 37.716 | 33.909 | 79.977 | 1.00 | 13.43 |
| ATOM | 3676 | SD  | MET | A | 462 | 36.053 | 34.635 | 80.074 | 1.00 | 19.12 |
| ATOM | 3677 | CE  | MET | A | 462 | 36.505 | 35.919 | 81.264 | 1.00 | 17.88 |
| ATOM | 3678 | N   | THR | A | 463 | 40.037 | 35.922 | 76.347 | 1.00 | 13.87 |
| ATOM | 3679 | CA  | THR | A | 463 | 41.004 | 36.860 | 75.849 | 1.00 | 12.21 |
| ATOM | 3680 | C   | THR | A | 463 | 40.675 | 38.339 | 75.910 | 1.00 | 16.34 |
| ATOM | 3681 | O   | THR | A | 463 | 41.365 | 39.106 | 76.567 | 1.00 | 16.05 |
| ATOM | 3682 | CB  | THR | A | 463 | 41.595 | 36.434 | 74.489 | 1.00 | 17.83 |
| ATOM | 3683 | OG1 | THR | A | 463 | 41.940 | 35.051 | 74.538 | 1.00 | 14.22 |
| ATOM | 3684 | CG2 | THR | A | 463 | 42.841 | 37.298 | 74.204 | 1.00 | 15.70 |
| ATOM | 3685 | N   | LEU | A | 464 | 39.679 | 38.762 | 75.136 | 1.00 | 14.21 |
| ATOM | 3686 | CA  | LEU | A | 464 | 39.262 | 40.154 | 75.060 | 1.00 | 13.52 |
| ATOM | 3687 | C   | LEU | A | 464 | 38.408 | 40.679 | 76.228 | 1.00 | 12.70 |
| ATOM | 3688 | O   | LEU | A | 464 | 38.259 | 41.881 | 76.442 | 1.00 | 15.39 |
| ATOM | 3689 | CB  | LEU | A | 464 | 38.508 | 40.348 | 73.725 | 1.00 | 13.87 |
| ATOM | 3690 | CG  | LEU | A | 464 | 39.363 | 40.009 | 72.495 | 1.00 | 18.04 |
| ATOM | 3691 | CD1 | LEU | A | 464 | 38.448 | 40.076 | 71.260 | 1.00 | 14.36 |
| ATOM | 3692 | CD2 | LEU | A | 464 | 40.490 | 41.054 | 72.345 | 1.00 | 17.86 |
| ATOM | 3693 | N   | THR | A | 465 | 37.808 | 39.770 | 76.979 | 1.00 | 11.81 |
| ATOM | 3694 | CA  | THR | A | 465 | 36.946 | 40.116 | 78.103 | 1.00 | 10.62 |
| ATOM | 3695 | C   | THR | A | 465 | 37.728 | 40.487 | 79.360 | 1.00 | 17.70 |
| ATOM | 3696 | O   | THR | A | 465 | 37.361 | 41.359 | 80.131 | 1.00 | 15.35 |
| ATOM | 3697 | CB  | THR | A | 465 | 35.996 | 38.934 | 78.368 | 1.00 | 12.56 |
| ATOM | 3698 | OG1 | THR | A | 465 | 35.209 | 38.765 | 77.199 | 1.00 | 16.68 |
| ATOM | 3699 | CG2 | THR | A | 465 | 35.075 | 39.241 | 79.545 | 1.00 | 17.17 |
| ATOM | 3700 | N   | ASN | A | 466 | 38.828 | 39.785 | 79.584 | 1.00 | 14.17 |
| ATOM | 3701 | CA  | ASN | A | 466 | 39.639 | 40.017 | 80.738 | 1.00 | 14.86 |
| ATOM | 3702 | C   | ASN | A | 466 | 39.933 | 41.491 | 81.017 | 1.00 | 16.02 |
| ATOM | 3703 | O   | ASN | A | 466 | 39.843 | 41.892 | 82.177 | 1.00 | 17.05 |
| ATOM | 3704 | CB  | ASN | A | 466 | 40.942 | 39.197 | 80.694 | 1.00 | 14.48 |
| ATOM | 3705 | CG  | ASN | A | 466 | 40.787 | 37.705 | 80.932 | 1.00 | 22.10 |
| ATOM | 3706 | OD1 | ASN | A | 466 | 41.539 | 36.878 | 80.386 | 1.00 | 21.72 |
| ATOM | 3707 | ND2 | ASN | A | 466 | 39.925 | 37.356 | 81.852 | 1.00 | 11.12 |
| ATOM | 3708 | N   | ALA | A | 467 | 40.313 | 42.307 | 80.012 | 1.00 | 16.17 |
| ATOM | 3709 | CA  | ALA | A | 467 | 40.614 | 43.704 | 80.336 | 1.00 | 16.10 |
| ATOM | 3710 | C   | ALA | A | 467 | 39.394 | 44.448 | 80.871 | 1.00 | 20.19 |
| ATOM | 3711 | O   | ALA | A | 467 | 39.488 | 45.363 | 81.722 | 1.00 | 17.63 |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 3712 | CB  | ALA | A | 467 | 41.159 | 44.411 | 79.118 | 1.00 | 14.71 |
| ATOM | 3713 | N   | CYS | A | 468 | 38.227 | 44.022 | 80.343 | 1.00 | 15.87 |
| ATOM | 3714 | CA  | CYS | A | 468 | 36.938 | 44.608 | 80.712 | 1.00 | 13.86 |
| ATOM | 3715 | C   | CYS | A | 468 | 36.609 | 44.369 | 82.167 | 1.00 | 15.16 |
| ATOM | 3716 | O   | CYS | A | 468 | 36.229 | 45.234 | 82.931 | 1.00 | 17.79 |
| ATOM | 3717 | CB  | CYS | A | 468 | 35.820 | 44.045 | 79.808 | 1.00 | 11.73 |
| ATOM | 3718 | SG  | CYS | A | 468 | 36.215 | 44.458 | 78.102 | 1.00 | 15.87 |
| ATOM | 3719 | N   | ILE | A | 469 | 36.811 | 43.145 | 82.571 | 1.00 | 13.83 |
| ATOM | 3720 | CA  | ILE | A | 469 | 36.531 | 42.747 | 83.941 | 1.00 | 11.80 |
| ATOM | 3721 | C   | ILE | A | 469 | 37.488 | 43.393 | 84.910 | 1.00 | 16.06 |
| ATOM | 3722 | O   | ILE | A | 469 | 37.076 | 43.848 | 85.970 | 1.00 | 18.22 |
| ATOM | 3723 | CB  | ILE | A | 469 | 36.659 | 41.230 | 84.042 | 1.00 | 15.30 |
| ATOM | 3724 | CG1 | ILE | A | 469 | 35.527 | 40.557 | 83.263 | 1.00 | 19.73 |
| ATOM | 3725 | CG2 | ILE | A | 469 | 36.688 | 40.791 | 85.497 | 1.00 | 11.46 |
| ATOM | 3726 | CD1 | ILE | A | 469 | 35.788 | 39.073 | 82.977 | 1.00 | 25.13 |
| ATOM | 3727 | N   | ALA | A | 470 | 38.776 | 43.375 | 84.572 | 1.00 | 12.77 |
| ATOM | 3728 | CA  | ALA | A | 470 | 39.729 | 43.967 | 85.475 | 1.00 | 11.93 |
| ATOM | 3729 | C   | ALA | A | 470 | 39.304 | 45.404 | 85.786 | 1.00 | 14.05 |
| ATOM | 3730 | O   | ALA | A | 470 | 39.264 | 45.860 | 86.941 | 1.00 | 15.14 |
| ATOM | 3731 | CB  | ALA | A | 470 | 41.078 | 43.982 | 84.759 | 1.00 | 12.54 |
| ATOM | 3732 | N   | LEU | A | 471 | 38.979 | 46.120 | 84.708 | 1.00 | 15.25 |
| ATOM | 3733 | CA  | LEU | A | 471 | 38.585 | 47.538 | 84.796 | 1.00 | 13.62 |
| ATOM | 3734 | C   | LEU | A | 471 | 37.257 | 47.792 | 85.510 | 1.00 | 17.64 |
| ATOM | 3735 | O   | LEU | A | 471 | 37.144 | 48.630 | 86.411 | 1.00 | 13.08 |
| ATOM | 3736 | CB  | LEU | A | 471 | 38.685 | 48.274 | 83.442 | 1.00 | 11.79 |
| ATOM | 3737 | CG  | LEU | A | 471 | 38.684 | 49.803 | 83.614 | 1.00 | 15.97 |
| ATOM | 3738 | CD1 | LEU | A | 471 | 39.855 | 50.262 | 84.497 | 1.00 | 12.47 |
| ATOM | 3739 | CD2 | LEU | A | 471 | 38.753 | 50.493 | 82.248 | 1.00 | 17.27 |
| ATOM | 3740 | N   | SER | A | 472 | 36.220 | 47.049 | 85.137 | 1.00 | 14.37 |
| ATOM | 3741 | CA  | SER | A | 472 | 34.963 | 47.264 | 85.808 | 1.00 | 11.84 |
| ATOM | 3742 | C   | SER | A | 472 | 35.082 | 46.900 | 87.284 | 1.00 | 18.13 |
| ATOM | 3743 | O   | SER | A | 472 | 34.533 | 47.581 | 88.145 | 1.00 | 16.29 |
| ATOM | 3744 | CB  | SER | A | 472 | 33.822 | 46.488 | 85.153 | 1.00 | 12.21 |
| ATOM | 3745 | OG  | SER | A | 472 | 34.090 | 45.121 | 85.240 | 1.00 | 18.74 |
| ATOM | 3746 | N   | GLN | A | 473 | 35.761 | 45.804 | 87.615 | 1.00 | 12.67 |
| ATOM | 3747 | CA  | GLN | A | 473 | 35.886 | 45.455 | 89.028 | 1.00 | 10.49 |
| ATOM | 3748 | C   | GLN | A | 473 | 36.615 | 46.538 | 89.813 | 1.00 | 12.50 |
| ATOM | 3749 | O   | GLN | A | 473 | 36.278 | 46.879 | 90.950 | 1.00 | 12.44 |
| ATOM | 3750 | CB  | GLN | A | 473 | 36.649 | 44.137 | 89.180 | 1.00 | 13.06 |
| ATOM | 3751 | CG  | GLN | A | 473 | 35.730 | 42.908 | 89.040 | 1.00 | 20.04 |
| ATOM | 3752 | CD  | GLN | A | 473 | 34.634 | 42.874 | 90.108 | 1.00 | 19.81 |
| ATOM | 3753 | OE1 | GLN | A | 473 | 34.917 | 42.605 | 91.270 | 1.00 | 30.46 |
| ATOM | 3754 | NE2 | GLN | A | 473 | 33.387 | 43.130 | 89.742 | 1.00 | 21.25 |
| ATOM | 3755 | N   | ARG | A | 474 | 37.656 | 47.087 | 89.183 | 1.00 | 14.11 |
| ATOM | 3756 | CA  | ARG | A | 474 | 38.400 | 48.158 | 89.868 | 1.00 | 17.39 |
| ATOM | 3757 | C   | ARG | A | 474 | 37.478 | 49.325 | 90.235 | 1.00 | 21.36 |
| ATOM | 3758 | O   | ARG | A | 474 | 37.577 | 49.922 | 91.304 | 1.00 | 18.76 |
| ATOM | 3759 | CB  | ARG | A | 474 | 39.532 | 48.719 | 89.034 | 1.00 | 11.27 |
| ATOM | 3760 | CG  | ARG | A | 474 | 40.786 | 47.842 | 89.038 | 1.00 | 17.88 |
| ATOM | 3761 | CD  | ARG | A | 474 | 41.727 | 48.283 | 87.928 | 1.00 | 21.70 |
| ATOM | 3762 | NE  | ARG | A | 474 | 42.122 | 49.665 | 88.177 | 1.00 | 19.49 |
| ATOM | 3763 | CZ  | ARG | A | 474 | 42.837 | 50.419 | 87.361 | 1.00 | 31.34 |
| ATOM | 3764 | NH1 | ARG | A | 474 | 43.239 | 49.918 | 86.190 | 1.00 | 25.99 |
| ATOM | 3765 | NH2 | ARG | A | 474 | 43.160 | 51.679 | 87.742 | 1.00 | 17.92 |
| ATOM | 3766 | N   | TRP | A | 475 | 36.602 | 49.686 | 89.306 | 1.00 | 14.64 |
| ATOM | 3767 | CA  | TRP | A | 475 | 35.683 | 50.774 | 89.542 | 1.00 | 13.85 |
| ATOM | 3768 | C   | TRP | A | 475 | 34.608 | 50.352 | 90.524 | 1.00 | 18.33 |
| ATOM | 3769 | O   | TRP | A | 475 | 34.250 | 51.076 | 91.430 | 1.00 | 15.30 |
| ATOM | 3770 | CB  | TRP | A | 475 | 35.033 | 51.236 | 88.235 | 1.00 | 13.65 |
| ATOM | 3771 | CG  | TRP | A | 475 | 35.867 | 52.222 | 87.479 | 1.00 | 14.81 |
| ATOM | 3772 | CD1 | TRP | A | 475 | 36.645 | 51.943 | 86.399 | 1.00 | 17.78 |



|      |      |     |     |   |     |        |        |         |      |       |
|------|------|-----|-----|---|-----|--------|--------|---------|------|-------|
| ATOM | 3773 | CD2 | TRP | A | 475 | 36.007 | 53.640 | 87.742  | 1.00 | 14.88 |
| ATOM | 3774 | NE1 | TRP | A | 475 | 37.284 | 53.090 | 85.976  | 1.00 | 18.25 |
| ATOM | 3775 | CE2 | TRP | A | 475 | 36.885 | 54.152 | 86.756  | 1.00 | 20.66 |
| ATOM | 3776 | CE3 | TRP | A | 475 | 35.464 | 54.518 | 88.694  | 1.00 | 15.98 |
| ATOM | 3777 | CZ2 | TRP | A | 475 | 37.243 | 55.511 | 86.714  | 1.00 | 19.78 |
| ATOM | 3778 | CZ3 | TRP | A | 475 | 35.839 | 55.853 | 88.665  | 1.00 | 18.27 |
| ATOM | 3779 | CH2 | TRP | A | 475 | 36.723 | 56.341 | 87.682  | 1.00 | 18.20 |
| ATOM | 3780 | N   | ILE | A | 476 | 34.081 | 49.157 | 90.362  | 1.00 | 15.43 |
| ATOM | 3781 | CA  | ILE | A | 476 | 33.027 | 48.713 | 91.251  | 1.00 | 15.88 |
| ATOM | 3782 | C   | ILE | A | 476 | 33.508 | 48.628 | 92.684  | 1.00 | 21.66 |
| ATOM | 3783 | O   | ILE | A | 476 | 32.742 | 48.833 | 93.614  | 1.00 | 20.18 |
| ATOM | 3784 | CB  | ILE | A | 476 | 32.498 | 47.354 | 90.775  | 1.00 | 16.74 |
| ATOM | 3785 | CG1 | ILE | A | 476 | 31.692 | 47.485 | 89.497  | 1.00 | 13.74 |
| ATOM | 3786 | CG2 | ILE | A | 476 | 31.697 | 46.620 | 91.844  | 1.00 | 17.08 |
| ATOM | 3787 | CD1 | ILE | A | 476 | 31.568 | 46.130 | 88.810  | 1.00 | 22.82 |
| ATOM | 3788 | N   | THR | A | 477 | 34.780 | 48.321 | 92.886  | 1.00 | 18.89 |
| ATOM | 3789 | CA  | THR | A | 477 | 35.286 | 48.193 | 94.256  | 1.00 | 15.92 |
| ATOM | 3790 | C   | THR | A | 477 | 36.151 | 49.355 | 94.708  | 1.00 | 17.65 |
| ATOM | 3791 | O   | THR | A | 477 | 36.711 | 49.333 | 95.792  | 1.00 | 17.49 |
| ATOM | 3792 | CB  | THR | A | 477 | 36.132 | 46.904 | 94.384  | 1.00 | 21.13 |
| ATOM | 3793 | OG1 | THR | A | 477 | 37.296 | 46.986 | 93.545  | 1.00 | 19.88 |
| ATOM | 3794 | CG2 | THR | A | 477 | 35.268 | 45.673 | 94.035  | 1.00 | 16.31 |
| ATOM | 3795 | N   | ALA | A | 478 | 36.302 | 50.369 | 93.884  | 1.00 | 18.44 |
| ATOM | 3796 | CA  | ALA | A | 478 | 37.131 | 51.548 | 94.191  | 1.00 | 16.94 |
| ATOM | 3797 | C   | ALA | A | 478 | 36.729 | 52.219 | 95.490  | 1.00 | 20.18 |
| ATOM | 3798 | O   | ALA | A | 478 | 35.552 | 52.233 | 95.863  | 1.00 | 19.40 |
| ATOM | 3799 | CB  | ALA | A | 478 | 37.017 | 52.608 | 93.077  | 1.00 | 15.66 |
| ATOM | 3800 | N   | LYS | A | 479 | 37.753 | 52.763 | 96.148  | 1.00 | 17.33 |
| ATOM | 3801 | CA  | LYS | A | 479 | 37.654 | 53.518 | 97.371  | 1.00 | 15.43 |
| ATOM | 3802 | C   | LYS | A | 479 | 38.196 | 54.907 | 97.115  | 1.00 | 19.77 |
| ATOM | 3803 | O   | LYS | A | 479 | 38.757 | 55.192 | 96.073  | 1.00 | 16.97 |
| ATOM | 3804 | CB  | LYS | A | 479 | 38.325 | 52.853 | 98.562  | 1.00 | 17.71 |
| ATOM | 3805 | CG  | LYS | A | 479 | 37.468 | 51.685 | 99.049  | 1.00 | 25.29 |
| ATOM | 3806 | CD  | LYS | A | 479 | 38.002 | 51.058 | 100.324 | 1.00 | 28.77 |
| ATOM | 3807 | CE  | LYS | A | 479 | 36.895 | 50.623 | 101.280 | 1.00 | 75.63 |
| ATOM | 3808 | NZ  | LYS | A | 479 | 36.090 | 49.481 | 100.815 | 1.00 | 66.83 |
| ATOM | 3809 | N   | GLU | A | 480 | 38.010 | 55.793 | 98.068  | 1.00 | 19.41 |
| ATOM | 3810 | CA  | GLU | A | 480 | 38.497 | 57.120 | 97.853  | 1.00 | 19.30 |
| ATOM | 3811 | C   | GLU | A | 480 | 39.933 | 57.069 | 97.387  | 1.00 | 21.25 |
| ATOM | 3812 | O   | GLU | A | 480 | 40.321 | 57.802 | 96.489  | 1.00 | 21.38 |
| ATOM | 3813 | CB  | GLU | A | 480 | 38.457 | 57.901 | 99.183  | 1.00 | 21.20 |
| ATOM | 3814 | CG  | GLU | A | 480 | 37.322 | 58.931 | 99.171  | 1.00 | 53.93 |
| ATOM | 3815 | CD  | GLU | A | 480 |        |        |         |      |       |



|      |      |     |     |   |     |        |        |        |      |        |
|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
| ATOM | 3834 | N   | LEU | A | 483 | 40.627 | 56.645 | 93.423 | 1.00 | 17.94  |
| ATOM | 3835 | CA  | LEU | A | 483 | 40.167 | 57.591 | 92.403 | 1.00 | 14.70  |
| ATOM | 3836 | C   | LEU | A | 483 | 41.214 | 58.319 | 91.581 | 1.00 | 21.17  |
| ATOM | 3837 | O   | LEU | A | 483 | 41.122 | 58.519 | 90.368 | 1.00 | 21.03  |
| ATOM | 3838 | CB  | LEU | A | 483 | 39.110 | 58.581 | 92.960 | 1.00 | 13.43  |
| ATOM | 3839 | CG  | LEU | A | 483 | 37.870 | 57.925 | 93.558 | 1.00 | 15.53  |
| ATOM | 3840 | CD1 | LEU | A | 483 | 36.970 | 59.020 | 94.114 | 1.00 | 19.32  |
| ATOM | 3841 | CD2 | LEU | A | 483 | 37.047 | 57.172 | 92.512 | 1.00 | 16.27  |
| ATOM | 3842 | N   | ASN | A | 484 | 42.220 | 58.761 | 92.289 | 1.00 | 19.63  |
| ATOM | 3843 | CA  | ASN | A | 484 | 43.274 | 59.541 | 91.713 | 1.00 | 19.74  |
| ATOM | 3844 | C   | ASN | A | 484 | 44.128 | 58.789 | 90.738 | 1.00 | 21.84  |
| ATOM | 3845 | O   | ASN | A | 484 | 44.723 | 59.343 | 89.827 | 1.00 | 20.30  |
| ATOM | 3846 | CB  | ASN | A | 484 | 44.110 | 60.036 | 92.891 | 1.00 | 34.83  |
| ATOM | 3847 | CG  | ASN | A | 484 | 45.382 | 60.719 | 92.449 | 1.00 | 100.00 |
| ATOM | 3848 | OD1 | ASN | A | 484 | 45.345 | 61.686 | 91.662 | 1.00 | 87.99  |
| ATOM | 3849 | ND2 | ASN | A | 484 | 46.510 | 60.200 | 92.946 | 1.00 | 100.00 |
| ATOM | 3850 | N   | SER | A | 485 | 44.183 | 57.510 | 90.918 | 1.00 | 17.69  |
| ATOM | 3851 | CA  | SER | A | 485 | 44.986 | 56.711 | 90.020 | 1.00 | 19.64  |
| ATOM | 3852 | C   | SER | A | 485 | 44.283 | 56.335 | 88.728 | 1.00 | 22.88  |
| ATOM | 3853 | O   | SER | A | 485 | 44.965 | 55.937 | 87.778 | 1.00 | 23.74  |
| ATOM | 3854 | CB  | SER | A | 485 | 45.543 | 55.508 | 90.752 | 1.00 | 26.03  |
| ATOM | 3855 | OG  | SER | A | 485 | 45.864 | 55.954 | 92.057 | 1.00 | 52.22  |
| ATOM | 3856 | N   | PHE | A | 486 | 42.948 | 56.451 | 88.650 | 1.00 | 15.68  |
| ATOM | 3857 | CA  | PHE | A | 486 | 42.367 | 56.105 | 87.371 | 1.00 | 17.12  |
| ATOM | 3858 | C   | PHE | A | 486 | 42.879 | 57.120 | 86.403 | 1.00 | 16.98  |
| ATOM | 3859 | O   | PHE | A | 486 | 43.165 | 58.236 | 86.812 | 1.00 | 15.87  |
| ATOM | 3860 | CB  | PHE | A | 486 | 40.827 | 56.088 | 87.376 | 1.00 | 18.47  |
| ATOM | 3861 | CG  | PHE | A | 486 | 40.270 | 54.950 | 88.181 | 1.00 | 17.85  |
| ATOM | 3862 | CD1 | PHE | A | 486 | 40.325 | 53.646 | 87.686 | 1.00 | 17.48  |
| ATOM | 3863 | CD2 | PHE | A | 486 | 39.669 | 55.169 | 89.423 | 1.00 | 19.85  |
| ATOM | 3864 | CE1 | PHE | A | 486 | 39.790 | 52.599 | 88.441 | 1.00 | 18.74  |
| ATOM | 3865 | CE2 | PHE | A | 486 | 39.119 | 54.139 | 90.189 | 1.00 | 19.10  |
| ATOM | 3866 | CZ  | PHE | A | 486 | 39.208 | 52.839 | 89.689 | 1.00 | 17.75  |
| ATOM | 3867 | N   | ASN | A | 487 | 42.965 | 56.744 | 85.140 | 1.00 | 16.22  |
| ATOM | 3868 | CA  | ASN | A | 487 | 43.499 | 57.636 | 84.141 | 1.00 | 20.09  |
| ATOM | 3869 | C   | ASN | A | 487 | 43.100 | 57.184 | 82.746 | 1.00 | 23.67  |
| ATOM | 3870 | O   | ASN | A | 487 | 42.770 | 56.024 | 82.522 | 1.00 | 22.60  |
| ATOM | 3871 | CB  | ASN | A | 487 | 45.058 | 57.575 | 84.255 | 1.00 | 21.63  |
| ATOM | 3872 | CG  | ASN | A | 487 | 45.776 | 58.616 | 83.415 | 1.00 | 32.80  |
| ATOM | 3873 | OD1 | ASN | A | 487 | 45.901 | 58.498 | 82.202 | 1.00 | 29.22  |
| ATOM | 3874 | ND2 | ASN | A | 487 | 46.159 | 59.725 | 84.021 | 1.00 | 31.52  |
| ATOM | 3875 | N   | ALA | A | 488 | 43.145 | 58.126 | 81.800 | 1.00 | 23.87  |
| ATOM | 3876 | CA  | ALA | A | 488 | 42.808 | 57.    |        |      |        |



|      |      |     |     |   |     |        |        |        |      |        |
|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
| ATOM | 3895 | N   | LEU | A | 491 | 42.309 | 53.262 | 79.180 | 1.00 | 14.42  |
| ATOM | 3896 | CA  | LEU | A | 491 | 41.571 | 52.910 | 77.971 | 1.00 | 18.63  |
| ATOM | 3897 | C   | LEU | A | 491 | 42.404 | 52.634 | 76.735 | 1.00 | 26.17  |
| ATOM | 3898 | O   | LEU | A | 491 | 41.863 | 52.350 | 75.689 | 1.00 | 23.53  |
| ATOM | 3899 | CB  | LEU | A | 491 | 40.626 | 54.065 | 77.600 | 1.00 | 16.48  |
| ATOM | 3900 | CG  | LEU | A | 491 | 39.793 | 54.553 | 78.786 | 1.00 | 17.62  |
| ATOM | 3901 | CD1 | LEU | A | 491 | 38.719 | 55.504 | 78.256 | 1.00 | 18.61  |
| ATOM | 3902 | CD2 | LEU | A | 491 | 39.164 | 53.341 | 79.481 | 1.00 | 10.99  |
| ATOM | 3903 | N   | LYS | A | 492 | 43.697 | 52.773 | 76.906 | 1.00 | 25.72  |
| ATOM | 3904 | CA  | LYS | A | 492 | 44.773 | 52.625 | 75.944 | 1.00 | 29.38  |
| ATOM | 3905 | C   | LYS | A | 492 | 44.601 | 51.464 | 74.987 | 1.00 | 26.62  |
| ATOM | 3906 | O   | LYS | A | 492 | 44.640 | 51.598 | 73.769 | 1.00 | 25.36  |
| ATOM | 3907 | CB  | LYS | A | 492 | 46.051 | 52.369 | 76.768 | 1.00 | 39.68  |
| ATOM | 3908 | CG  | LYS | A | 492 | 47.400 | 52.731 | 76.164 | 1.00 | 74.03  |
| ATOM | 3909 | CD  | LYS | A | 492 | 48.535 | 52.573 | 77.175 | 1.00 | 92.88  |
| ATOM | 3910 | CE  | LYS | A | 492 | 49.162 | 51.184 | 77.249 | 1.00 | 100.00 |
| ATOM | 3911 | NZ  | LYS | A | 492 | 50.629 | 51.214 | 77.397 | 1.00 | 100.00 |
| ATOM | 3912 | N   | ASP | A | 493 | 44.504 | 50.271 | 75.514 | 1.00 | 22.05  |
| ATOM | 3913 | CA  | ASP | A | 493 | 44.400 | 49.213 | 74.525 | 1.00 | 25.28  |
| ATOM | 3914 | C   | ASP | A | 493 | 43.008 | 48.604 | 74.421 | 1.00 | 31.85  |
| ATOM | 3915 | O   | ASP | A | 493 | 42.844 | 47.411 | 74.178 | 1.00 | 31.64  |
| ATOM | 3916 | CB  | ASP | A | 493 | 45.414 | 48.126 | 74.874 | 1.00 | 30.29  |
| ATOM | 3917 | CG  | ASP | A | 493 | 46.803 | 48.680 | 74.973 | 1.00 | 47.27  |
| ATOM | 3918 | OD1 | ASP | A | 493 | 47.322 | 49.280 | 74.036 | 1.00 | 49.99  |
| ATOM | 3919 | OD2 | ASP | A | 493 | 47.334 | 48.481 | 76.167 | 1.00 | 45.03  |
| ATOM | 3920 | N   | LEU | A | 494 | 41.989 | 49.430 | 74.622 | 1.00 | 23.95  |
| ATOM | 3921 | CA  | LEU | A | 494 | 40.633 | 48.920 | 74.576 | 1.00 | 19.08  |
| ATOM | 3922 | C   | LEU | A | 494 | 39.939 | 49.350 | 73.295 | 1.00 | 21.27  |
| ATOM | 3923 | O   | LEU | A | 494 | 39.960 | 50.537 | 72.963 | 1.00 | 22.24  |
| ATOM | 3924 | CB  | LEU | A | 494 | 39.833 | 49.421 | 75.800 | 1.00 | 16.85  |
| ATOM | 3925 | CG  | LEU | A | 494 | 40.346 | 48.949 | 77.145 | 1.00 | 19.46  |
| ATOM | 3926 | CD1 | LEU | A | 494 | 39.307 | 49.363 | 78.182 | 1.00 | 18.39  |
| ATOM | 3927 | CD2 | LEU | A | 494 | 40.511 | 47.422 | 77.183 | 1.00 | 20.77  |
| ATOM | 3928 | N   | SER | A | 495 | 39.320 | 48.401 | 72.573 | 1.00 | 17.36  |
| ATOM | 3929 | CA  | SER | A | 495 | 38.594 | 48.790 | 71.382 | 1.00 | 16.04  |
| ATOM | 3930 | C   | SER | A | 495 | 37.256 | 49.395 | 71.854 | 1.00 | 16.87  |
| ATOM | 3931 | O   | SER | A | 495 | 36.902 | 49.328 | 73.042 | 1.00 | 13.30  |
| ATOM | 3932 | CB  | SER | A | 495 | 38.253 | 47.547 | 70.576 | 1.00 | 16.67  |
| ATOM | 3933 | OG  | SER | A | 495 | 37.477 | 46.701 | 71.422 | 1.00 | 17.37  |
| ATOM | 3934 | N   | SER | A | 496 | 36.496 | 49.950 | 70.922 | 1.00 | 14.14  |
| ATOM | 3935 | CA  | SER | A | 496 | 35.200 | 50.501 | 71.254 | 1.00 | 16.64  |
| ATOM | 3936 | C   | SER | A | 496 | 34.316 | 49.365 | 71.794 | 1.00 | 17.90  |
| ATOM | 3937 | O   | SER | A | 496 | 33.    |        |        |      |        |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 3956 | CD  | GLN | A | 498 | 39.101 | 44.938 | 74.454 | 1.00 | 21.92 |
| ATOM | 3957 | OE1 | GLN | A | 498 | 39.746 | 45.833 | 73.897 | 1.00 | 18.12 |
| ATOM | 3958 | NE2 | GLN | A | 498 | 39.685 | 43.957 | 75.117 | 1.00 | 11.55 |
| ATOM | 3959 | N   | LEU | A | 499 | 35.200 | 48.942 | 75.490 | 1.00 | 16.63 |
| ATOM | 3960 | CA  | LEU | A | 499 | 34.712 | 50.095 | 76.273 | 1.00 | 18.30 |
| ATOM | 3961 | C   | LEU | A | 499 | 33.222 | 49.848 | 76.647 | 1.00 | 18.08 |
| ATOM | 3962 | O   | LEU | A | 499 | 32.711 | 50.004 | 77.782 | 1.00 | 14.69 |
| ATOM | 3963 | CB  | LEU | A | 499 | 34.719 | 51.296 | 75.293 | 1.00 | 19.02 |
| ATOM | 3964 | CG  | LEU | A | 499 | 35.650 | 52.421 | 75.677 | 1.00 | 28.28 |
| ATOM | 3965 | CD1 | LEU | A | 499 | 36.768 | 51.856 | 76.527 | 1.00 | 27.69 |
| ATOM | 3966 | CD2 | LEU | A | 499 | 36.210 | 53.135 | 74.448 | 1.00 | 31.77 |
| ATOM | 3967 | N   | ASN | A | 500 | 32.491 | 49.430 | 75.610 | 1.00 | 11.59 |
| ATOM | 3968 | CA  | ASN | A | 500 | 31.084 | 49.123 | 75.748 | 1.00 | 10.98 |
| ATOM | 3969 | C   | ASN | A | 500 | 30.844 | 48.021 | 76.775 | 1.00 | 11.55 |
| ATOM | 3970 | O   | ASN | A | 500 | 29.989 | 48.125 | 77.656 | 1.00 | 13.43 |
| ATOM | 3971 | CB  | ASN | A | 500 | 30.530 | 48.735 | 74.355 | 1.00 | 11.90 |
| ATOM | 3972 | CG  | ASN | A | 500 | 29.020 | 48.504 | 74.328 | 1.00 | 26.05 |
| ATOM | 3973 | OD1 | ASN | A | 500 | 28.208 | 49.304 | 74.815 | 1.00 | 19.55 |
| ATOM | 3974 | ND2 | ASN | A | 500 | 28.607 | 47.387 | 73.759 | 1.00 | 21.02 |
| ATOM | 3975 | N   | GLU | A | 501 | 31.601 | 46.927 | 76.633 | 1.00 | 11.18 |
| ATOM | 3976 | CA  | GLU | A | 501 | 31.471 | 45.787 | 77.537 | 1.00 | 11.00 |
| ATOM | 3977 | C   | GLU | A | 501 | 31.859 | 46.184 | 78.954 | 1.00 | 14.40 |
| ATOM | 3978 | O   | GLU | A | 501 | 31.266 | 45.757 | 79.930 | 1.00 | 13.70 |
| ATOM | 3979 | CB  | GLU | A | 501 | 32.286 | 44.574 | 77.022 | 1.00 | 13.23 |
| ATOM | 3980 | CG  | GLU | A | 501 | 32.328 | 43.425 | 78.064 | 1.00 | 12.24 |
| ATOM | 3981 | CD  | GLU | A | 501 | 30.930 | 42.880 | 78.253 | 1.00 | 20.51 |
| ATOM | 3982 | OE1 | GLU | A | 501 | 30.040 | 43.113 | 77.452 | 1.00 | 18.75 |
| ATOM | 3983 | OE2 | GLU | A | 501 | 30.747 | 42.158 | 79.338 | 1.00 | 16.17 |
| ATOM | 3984 | N   | PHE | A | 502 | 32.876 | 47.051 | 79.080 | 1.00 | 10.99 |
| ATOM | 3985 | CA  | PHE | A | 502 | 33.281 | 47.530 | 80.382 | 1.00 | 12.47 |
| ATOM | 3986 | C   | PHE | A | 502 | 32.095 | 48.241 | 81.068 | 1.00 | 12.80 |
| ATOM | 3987 | O   | PHE | A | 502 | 31.733 | 48.062 | 82.230 | 1.00 | 11.74 |
| ATOM | 3988 | CB  | PHE | A | 502 | 34.498 | 48.490 | 80.167 | 1.00 | 14.11 |
| ATOM | 3989 | CG  | PHE | A | 502 | 34.641 | 49.500 | 81.265 | 1.00 | 11.76 |
| ATOM | 3990 | CD1 | PHE | A | 502 | 34.958 | 49.120 | 82.570 | 1.00 | 9.77  |
| ATOM | 3991 | CD2 | PHE | A | 502 | 34.363 | 50.847 | 81.040 | 1.00 | 17.45 |
| ATOM | 3992 | CE1 | PHE | A | 502 | 35.059 | 50.053 | 83.605 | 1.00 | 12.88 |
| ATOM | 3993 | CE2 | PHE | A | 502 | 34.443 | 51.799 | 82.063 | 1.00 | 20.32 |
| ATOM | 3994 | CZ  | PHE | A | 502 | 34.812 | 51.406 | 83.350 | 1.00 | 16.55 |
| ATOM | 3995 | N   | LEU | A | 503 | 31.470 | 49.100 | 80.286 | 1.00 | 10.48 |
| ATOM | 3996 | CA  | LEU | A | 503 | 30.342 | 49.835 | 80.759 | 1.00 | 11.84 |
| ATOM | 3997 | C   | LEU | A | 503 | 29.184 | 48.917 | 81.089 | 1.00 | 11.65 |
| ATOM | 3998 | O   | LEU | A | 503 | 28.531 | 49.077 | 82.110 | 1.00 | 14.41 |
| ATOM | 3999 | CB  | LEU | A | 503 | 29.974 | 50.854 | 79.668 | 1.00 | 12.15 |
| ATOM | 4000 | CG  | LEU | A | 503 | 30.872 | 52.105 | 79.668 | 1.00 | 12.97 |
| ATOM | 4001 | CD1 | LEU | A | 503 | 30.572 | 52.957 | 78.438 | 1.00 | 9.62  |
| ATOM | 4002 | CD2 | LEU | A | 503 | 30.614 | 52.935 | 80.936 | 1.00 | 14.08 |
| ATOM | 4003 | N   | ALA | A | 504 | 28.947 | 47.910 | 80.248 | 1.00 | 12.65 |
| ATOM | 4004 | CA  | ALA | A | 504 | 27.850 | 46.977 | 80.499 | 1.00 | 8.77  |
| ATOM | 4005 | C   | ALA | A | 504 | 28.038 | 46.282 | 81.812 | 1.00 | 12.09 |
| ATOM | 4006 | O   | ALA | A | 504 | 27.118 | 46.081 | 82.598 | 1.00 | 10.26 |
| ATOM | 4007 | CB  | ALA | A | 504 | 27.742 | 45.965 | 79.370 | 1.00 | 7.47  |
| ATOM | 4008 | N   | GLN | A | 505 | 29.280 | 45.900 | 82.035 | 1.00 | 12.47 |
| ATOM | 4009 | CA  | GLN | A | 505 | 29.609 | 45.209 | 83.271 | 1.00 | 12.94 |
| ATOM | 4010 | C   | GLN | A | 505 | 29.424 | 46.144 | 84.484 | 1.00 | 14.71 |
| ATOM | 4011 | O   | GLN | A | 505 | 28.902 | 45.773 | 85.566 | 1.00 | 13.04 |
| ATOM | 4012 | CB  | GLN | A | 505 | 31.068 | 44.689 | 83.183 | 1.00 | 14.37 |
| ATOM | 4013 | CG  | GLN | A | 505 | 31.243 | 43.520 | 82.174 | 1.00 | 17.48 |
| ATOM | 4014 | CD  | GLN | A | 505 | 32.693 | 43.054 | 82.089 | 1.00 | 20.84 |
| ATOM | 4015 | OE1 | GLN | A | 505 | 33.556 | 43.462 | 82.890 | 1.00 | 21.65 |
| ATOM | 4016 | NE2 | GLN | A | 505 | 32.990 | 42.221 | 81.096 | 1.00 | 16.13 |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 4017 | N   | THR | A | 506 | 29.862 | 47.389 | 84.298 | 1.00 | 13.56 |
| ATOM | 4018 | CA  | THR | A | 506 | 29.749 | 48.348 | 85.373 | 1.00 | 15.13 |
| ATOM | 4019 | C   | THR | A | 506 | 28.280 | 48.610 | 85.714 | 1.00 | 17.30 |
| ATOM | 4020 | O   | THR | A | 506 | 27.835 | 48.662 | 86.879 | 1.00 | 13.71 |
| ATOM | 4021 | CB  | THR | A | 506 | 30.561 | 49.613 | 85.043 | 1.00 | 13.74 |
| ATOM | 4022 | OG1 | THR | A | 506 | 31.903 | 49.243 | 84.853 | 1.00 | 13.66 |
| ATOM | 4023 | CG2 | THR | A | 506 | 30.542 | 50.538 | 86.242 | 1.00 | 16.98 |
| ATOM | 4024 | N   | LEU | A | 507 | 27.532 | 48.734 | 84.636 | 1.00 | 15.17 |
| ATOM | 4025 | CA  | LEU | A | 507 | 26.109 | 49.007 | 84.748 | 1.00 | 15.46 |
| ATOM | 4026 | C   | LEU | A | 507 | 25.391 | 47.944 | 85.517 | 1.00 | 15.53 |
| ATOM | 4027 | O   | LEU | A | 507 | 24.464 | 48.230 | 86.256 | 1.00 | 14.11 |
| ATOM | 4028 | CB  | LEU | A | 507 | 25.476 | 49.185 | 83.351 | 1.00 | 16.26 |
| ATOM | 4029 | CG  | LEU | A | 507 | 24.017 | 49.581 | 83.374 | 1.00 | 17.96 |
| ATOM | 4030 | CD1 | LEU | A | 507 | 23.801 | 50.929 | 84.087 | 1.00 | 12.71 |
| ATOM | 4031 | CD2 | LEU | A | 507 | 23.550 | 49.633 | 81.923 | 1.00 | 13.10 |
| ATOM | 4032 | N   | GLN | A | 508 | 25.802 | 46.696 | 85.343 | 1.00 | 14.24 |
| ATOM | 4033 | CA  | GLN | A | 508 | 25.145 | 45.630 | 86.077 | 1.00 | 11.70 |
| ATOM | 4034 | C   | GLN | A | 508 | 25.264 | 45.846 | 87.581 | 1.00 | 19.07 |
| ATOM | 4035 | O   | GLN | A | 508 | 24.521 | 45.269 | 88.354 | 1.00 | 16.98 |
| ATOM | 4036 | CB  | GLN | A | 508 | 25.736 | 44.246 | 85.745 | 1.00 | 11.79 |
| ATOM | 4037 | CG  | GLN | A | 508 | 25.402 | 43.722 | 84.334 | 1.00 | 17.73 |
| ATOM | 4038 | CD  | GLN | A | 508 | 25.860 | 42.282 | 84.204 | 1.00 | 20.08 |
| ATOM | 4039 | OE1 | GLN | A | 508 | 26.960 | 41.972 | 84.695 | 1.00 | 23.98 |
| ATOM | 4040 | NE2 | GLN | A | 508 | 25.048 | 41.402 | 83.594 | 1.00 | 15.23 |
| ATOM | 4041 | N   | ARG | A | 509 | 26.217 | 46.639 | 88.053 | 1.00 | 17.16 |
| ATOM | 4042 | CA  | ARG | A | 509 | 26.332 | 46.847 | 89.498 | 1.00 | 12.26 |
| ATOM | 4043 | C   | ARG | A | 509 | 25.960 | 48.279 | 89.899 | 1.00 | 17.09 |
| ATOM | 4044 | O   | ARG | A | 509 | 26.379 | 48.778 | 90.948 | 1.00 | 18.12 |
| ATOM | 4045 | CB  | ARG | A | 509 | 27.741 | 46.537 | 90.036 | 1.00 | 12.59 |
| ATOM | 4046 | CG  | ARG | A | 509 | 28.095 | 45.097 | 89.784 | 1.00 | 17.56 |
| ATOM | 4047 | CD  | ARG | A | 509 | 27.422 | 44.228 | 90.829 | 1.00 | 25.37 |
| ATOM | 4048 | NE  | ARG | A | 509 | 28.134 | 44.270 | 92.117 | 1.00 | 81.24 |
| ATOM | 4049 | CZ  | ARG | A | 509 | 29.377 | 43.822 | 92.417 | 1.00 | 88.85 |
| ATOM | 4050 | NH1 | ARG | A | 509 | 30.235 | 43.233 | 91.555 | 1.00 | 63.02 |
| ATOM | 4051 | NH2 | ARG | A | 509 | 29.779 | 43.978 | 93.676 | 1.00 | 42.33 |
| ATOM | 4052 | N   | ALA | A | 510 | 25.162 | 48.958 | 89.088 | 1.00 | 14.89 |
| ATOM | 4053 | CA  | ALA | A | 510 | 24.782 | 50.321 | 89.428 | 1.00 | 13.02 |
| ATOM | 4054 | C   | ALA | A | 510 | 23.824 | 50.270 | 90.594 | 1.00 | 22.66 |
| ATOM | 4055 | O   | ALA | A | 510 | 23.176 | 49.243 | 90.747 | 1.00 | 21.57 |
| ATOM | 4056 | CB  | ALA | A | 510 | 24.166 | 51.066 | 88.248 | 1.00 | 13.60 |
| ATOM | 4057 | N   | PRO | A | 511 | 23.755 | 51.340 | 91.417 | 1.00 | 20.55 |
| ATOM | 4058 | CA  | PRO | A | 511 | 24.521 | 52.568 | 91.190 | 1.00 | 16.50 |
| ATOM | 4059 | C   | PRO | A | 511 | 25.912 |        |        |      |       |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 4078 | CD  | PRO | A | 513 | 29.960 | 54.270 | 93.987 | 1.00 | 17.15 |
| ATOM | 4079 | N   | LEU | A | 514 | 28.154 | 58.573 | 93.341 | 1.00 | 19.37 |
| ATOM | 4080 | CA  | LEU | A | 514 | 28.155 | 59.712 | 92.431 | 1.00 | 20.71 |
| ATOM | 4081 | C   | LEU | A | 514 | 29.567 | 60.240 | 92.151 | 1.00 | 22.73 |
| ATOM | 4082 | O   | LEU | A | 514 | 29.934 | 60.486 | 90.991 | 1.00 | 20.91 |
| ATOM | 4083 | CB  | LEU | A | 514 | 27.209 | 60.816 | 92.955 | 1.00 | 19.46 |
| ATOM | 4084 | CG  | LEU | A | 514 | 27.173 | 62.058 | 92.077 | 1.00 | 23.47 |
| ATOM | 4085 | CD1 | LEU | A | 514 | 26.650 | 61.694 | 90.681 | 1.00 | 21.60 |
| ATOM | 4086 | CD2 | LEU | A | 514 | 26.275 | 63.087 | 92.767 | 1.00 | 19.09 |
| ATOM | 4087 | N   | GLY | A | 515 | 30.353 | 60.384 | 93.236 | 1.00 | 19.02 |
| ATOM | 4088 | CA  | GLY | A | 515 | 31.711 | 60.866 | 93.104 | 1.00 | 16.33 |
| ATOM | 4089 | C   | GLY | A | 515 | 32.489 | 60.000 | 92.121 | 1.00 | 20.68 |
| ATOM | 4090 | O   | GLY | A | 515 | 33.336 | 60.489 | 91.363 | 1.00 | 17.47 |
| ATOM | 4091 | N   | HIS | A | 516 | 32.199 | 58.691 | 92.105 | 1.00 | 16.69 |
| ATOM | 4092 | CA  | HIS | A | 516 | 32.961 | 57.829 | 91.206 | 1.00 | 16.67 |
| ATOM | 4093 | C   | HIS | A | 516 | 32.629 | 58.092 | 89.762 | 1.00 | 16.39 |
| ATOM | 4094 | O   | HIS | A | 516 | 33.485 | 58.094 | 88.886 | 1.00 | 13.40 |
| ATOM | 4095 | CB  | HIS | A | 516 | 32.781 | 56.335 | 91.479 | 1.00 | 16.85 |
| ATOM | 4096 | CG  | HIS | A | 516 | 33.328 | 55.909 | 92.786 | 1.00 | 23.07 |
| ATOM | 4097 | ND1 | HIS | A | 516 | 33.586 | 56.811 | 93.804 | 1.00 | 27.10 |
| ATOM | 4098 | CD2 | HIS | A | 516 | 33.691 | 54.664 | 93.219 | 1.00 | 26.55 |
| ATOM | 4099 | CE1 | HIS | A | 516 | 34.067 | 56.096 | 94.831 | 1.00 | 27.40 |
| ATOM | 4100 | NE2 | HIS | A | 516 | 34.144 | 54.803 | 94.514 | 1.00 | 26.59 |
| ATOM | 4101 | N   | ILE | A | 517 | 31.349 | 58.288 | 89.534 | 1.00 | 14.76 |
| ATOM | 4102 | CA  | ILE | A | 517 | 30.887 | 58.520 | 88.189 | 1.00 | 15.71 |
| ATOM | 4103 | C   | ILE | A | 517 | 31.444 | 59.817 | 87.666 | 1.00 | 13.62 |
| ATOM | 4104 | O   | ILE | A | 517 | 31.851 | 59.960 | 86.511 | 1.00 | 13.02 |
| ATOM | 4105 | CB  | ILE | A | 517 | 29.350 | 58.408 | 88.144 | 1.00 | 20.46 |
| ATOM | 4106 | CG1 | ILE | A | 517 | 28.925 | 56.989 | 88.555 | 1.00 | 23.97 |
| ATOM | 4107 | CG2 | ILE | A | 517 | 28.793 | 58.653 | 86.750 | 1.00 | 19.51 |
| ATOM | 4108 | CD1 | ILE | A | 517 | 29.636 | 55.831 | 87.826 | 1.00 | 21.92 |
| ATOM | 4109 | N   | LYS | A | 518 | 31.433 | 60.804 | 88.549 | 1.00 | 13.76 |
| ATOM | 4110 | CA  | LYS | A | 518 | 32.004 | 62.082 | 88.137 | 1.00 | 12.83 |
| ATOM | 4111 | C   | LYS | A | 518 | 33.487 | 61.877 | 87.759 | 1.00 | 17.13 |
| ATOM | 4112 | O   | LYS | A | 518 | 33.971 | 62.371 | 86.745 | 1.00 | 14.95 |
| ATOM | 4113 | CB  | LYS | A | 518 | 31.858 | 63.092 | 89.279 | 1.00 | 12.59 |
| ATOM | 4114 | CG  | LYS | A | 518 | 30.392 | 63.447 | 89.416 | 1.00 | 15.77 |
| ATOM | 4115 | CD  | LYS | A | 518 | 30.169 | 64.528 | 90.446 | 1.00 | 25.59 |
| ATOM | 4116 | CE  | LYS | A | 518 | 28.743 | 65.047 | 90.425 | 1.00 | 26.22 |
| ATOM | 4117 | NZ  | LYS | A | 518 | 28.669 | 66.440 | 90.886 | 1.00 | 26.75 |
| ATOM | 4118 | N   | ARG | A | 519 | 34.237 | 61.144 | 88.604 | 1.00 | 15.99 |
| ATOM | 4119 | CA  | ARG | A | 519 | 35.647 | 60.914 | 88.321 | 1.00 | 13.25 |
| ATOM | 4120 | C   | ARG | A | 519 | 35.803 | 60.213 | 86.998 | 1.00 | 16.26 |
| ATOM | 4121 | O   | ARG | A | 519 | 36.679 | 60.478 | 86.216 | 1.00 | 13.50 |
| ATOM | 4122 | CB  | ARG | A | 519 | 36.265 | 60.075 | 89.423 | 1.00 | 14.16 |
| ATOM | 4123 | CG  | ARG | A | 519 | 37.741 | 59.741 | 89.216 | 1.00 | 13.79 |
| ATOM | 4124 | CD  | ARG | A | 519 | 38.685 | 60.955 | 89.134 | 1.00 | 22.42 |
| ATOM | 4125 | NE  | ARG | A | 519 | 40.127 | 60.613 | 89.069 | 1.00 | 17.77 |
| ATOM | 4126 | CZ  | ARG | A | 519 | 41.035 | 61.432 | 88.570 | 1.00 | 19.26 |
| ATOM | 4127 | NH1 | ARG | A | 519 | 40.692 | 62.640 | 88.087 | 1.00 | 18.57 |
| ATOM | 4128 | NH2 | ARG | A | 519 | 42.289 | 61.014 | 88.549 | 1.00 | 17.51 |
| ATOM | 4129 | N   | MET | A | 520 | 34.897 | 59.292 | 86.743 | 1.00 | 13.85 |
| ATOM | 4130 | CA  | MET | A | 520 | 34.944 | 58.548 | 85.514 | 1.00 | 13.32 |
| ATOM | 4131 | C   | MET | A | 520 | 34.803 | 59.460 | 84.299 | 1.00 | 16.61 |
| ATOM | 4132 | O   | MET | A | 520 | 35.461 | 59.286 | 83.279 | 1.00 | 15.39 |
| ATOM | 4133 | CB  | MET | A | 520 | 33.860 | 57.425 | 85.585 | 1.00 | 15.92 |
| ATOM | 4134 | CG  | MET | A | 520 | 33.887 | 56.502 | 84.369 | 1.00 | 16.73 |
| ATOM | 4135 | SD  | MET | A | 520 | 32.699 | 55.131 | 84.463 | 1.00 | 19.40 |
| ATOM | 4136 | CE  | MET | A | 520 | 33.250 | 54.267 | 85.942 | 1.00 | 17.31 |
| ATOM | 4137 | N   | GLN | A | 521 | 33.919 | 60.449 | 84.358 | 1.00 | 10.96 |
| ATOM | 4138 | CA  | GLN | A | 521 | 33.800 | 61.336 | 83.205 | 1.00 | 10.25 |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 4139 | C   | GLN | A | 521 | 35.105 | 62.160 | 83.122 | 1.00 | 14.21 |
| ATOM | 4140 | O   | GLN | A | 521 | 35.684 | 62.487 | 82.073 | 1.00 | 11.43 |
| ATOM | 4141 | CB  | GLN | A | 521 | 32.548 | 62.237 | 83.376 | 1.00 | 9.22  |
| ATOM | 4142 | CG  | GLN | A | 521 | 32.547 | 63.519 | 82.503 | 1.00 | 12.68 |
| ATOM | 4143 | CD  | GLN | A | 521 | 32.758 | 63.301 | 81.025 | 1.00 | 18.23 |
| ATOM | 4144 | OE1 | GLN | A | 521 | 33.271 | 64.187 | 80.309 | 1.00 | 20.20 |
| ATOM | 4145 | NE2 | GLN | A | 521 | 32.453 | 62.102 | 80.554 | 1.00 | 10.43 |
| ATOM | 4146 | N   | GLU | A | 522 | 35.608 | 62.524 | 84.295 | 1.00 | 15.29 |
| ATOM | 4147 | CA  | GLU | A | 522 | 36.816 | 63.335 | 84.345 | 1.00 | 14.86 |
| ATOM | 4148 | C   | GLU | A | 522 | 38.026 | 62.632 | 83.702 | 1.00 | 24.87 |
| ATOM | 4149 | O   | GLU | A | 522 | 38.848 | 63.232 | 82.990 | 1.00 | 19.95 |
| ATOM | 4150 | CB  | GLU | A | 522 | 37.068 | 63.573 | 85.820 | 1.00 | 15.93 |
| ATOM | 4151 | CG  | GLU | A | 522 | 38.175 | 64.573 | 86.121 | 1.00 | 34.79 |
| ATOM | 4152 | CD  | GLU | A | 522 | 38.013 | 64.959 | 87.556 | 1.00 | 61.54 |
| ATOM | 4153 | OE1 | GLU | A | 522 | 38.436 | 64.271 | 88.466 | 1.00 | 24.02 |
| ATOM | 4154 | OE2 | GLU | A | 522 | 37.252 | 66.014 | 87.710 | 1.00 | 60.58 |
| ATOM | 4155 | N   | VAL | A | 523 | 38.179 | 61.338 | 83.966 | 1.00 | 17.81 |
| ATOM | 4156 | CA  | VAL | A | 523 | 39.302 | 60.635 | 83.392 | 1.00 | 17.49 |
| ATOM | 4157 | C   | VAL | A | 523 | 39.081 | 60.051 | 81.994 | 1.00 | 17.20 |
| ATOM | 4158 | O   | VAL | A | 523 | 40.038 | 59.940 | 81.230 | 1.00 | 22.12 |
| ATOM | 4159 | CB  | VAL | A | 523 | 39.952 | 59.621 | 84.340 | 1.00 | 18.80 |
| ATOM | 4160 | CG1 | VAL | A | 523 | 40.427 | 60.324 | 85.613 | 1.00 | 18.67 |
| ATOM | 4161 | CG2 | VAL | A | 523 | 38.957 | 58.522 | 84.717 | 1.00 | 17.30 |
| ATOM | 4162 | N   | TYR | A | 524 | 37.851 | 59.676 | 81.633 | 1.00 | 13.33 |
| ATOM | 4163 | CA  | TYR | A | 524 | 37.638 | 59.045 | 80.331 | 1.00 | 12.09 |
| ATOM | 4164 | C   | TYR | A | 524 | 36.842 | 59.839 | 79.321 | 1.00 | 19.77 |
| ATOM | 4165 | O   | TYR | A | 524 | 36.720 | 59.417 | 78.179 | 1.00 | 17.94 |
| ATOM | 4166 | CB  | TYR | A | 524 | 36.961 | 57.656 | 80.463 | 1.00 | 13.83 |
| ATOM | 4167 | CG  | TYR | A | 524 | 37.615 | 56.667 | 81.421 | 1.00 | 14.86 |
| ATOM | 4168 | CD1 | TYR | A | 524 | 38.999 | 56.608 | 81.574 | 1.00 | 13.07 |
| ATOM | 4169 | CD2 | TYR | A | 524 | 36.832 | 55.761 | 82.146 | 1.00 | 19.57 |
| ATOM | 4170 | CE1 | TYR | A | 524 | 39.592 | 55.704 | 82.460 | 1.00 | 18.13 |
| ATOM | 4171 | CE2 | TYR | A | 524 | 37.403 | 54.832 | 83.019 | 1.00 | 18.46 |
| ATOM | 4172 | CZ  | TYR | A | 524 | 38.790 | 54.813 | 83.181 | 1.00 | 17.58 |
| ATOM | 4173 | OH  | TYR | A | 524 | 39.360 | 53.937 | 84.087 | 1.00 | 16.81 |
| ATOM | 4174 | N   | ASN | A | 525 | 36.235 | 60.940 | 79.753 | 1.00 | 20.91 |
| ATOM | 4175 | CA  | ASN | A | 525 | 35.435 | 61.755 | 78.865 | 1.00 | 16.88 |
| ATOM | 4176 | C   | ASN | A | 525 | 34.488 | 60.923 | 78.018 | 1.00 | 18.05 |
| ATOM | 4177 | O   | ASN | A | 525 | 34.450 | 61.014 | 76.789 | 1.00 | 15.92 |
| ATOM | 4178 | CB  | ASN | A | 525 | 36.361 | 62.615 | 78.002 | 1.00 | 13.81 |
| ATOM | 4179 | CG  | ASN | A | 525 | 35.680 | 63.751 | 77.259 | 1.00 | 18.94 |
| ATOM | 4180 | OD1 | ASN | A | 525 | 36.243 | 64.268 | 76.280 | 1.00 | 18.98 |
| ATOM | 4181 | ND2 | ASN | A | 525 | 34.502 | 64.169 | 77.693 | 1.00 | 14.31 |
| ATOM | 4182 | N   | PHE | A | 526 | 33.659 | 60.120 | 78.683 | 1.00 | 14.70 |
| ATOM | 4183 | CA  | PHE | A | 526 | 32.676 | 59.337 | 77.947 | 1.00 | 12.71 |
| ATOM | 4184 | C   | PHE | A | 526 | 31.596 | 60.234 | 77.380 | 1.00 | 16.60 |
| ATOM | 4185 | O   | PHE | A | 526 | 30.891 | 59.866 | 76.439 | 1.00 | 15.88 |
| ATOM | 4186 | CB  | PHE | A | 526 | 32.038 | 58.303 | 78.876 | 1.00 | 14.35 |
| ATOM | 4187 | CG  | PHE | A | 526 | 32.957 | 57.130 | 79.130 | 1.00 | 15.85 |
| ATOM | 4188 | CD1 | PHE | A | 526 | 33.895 | 56.735 | 78.175 | 1.00 | 19.68 |
| ATOM | 4189 | CD2 | PHE | A | 526 | 32.876 | 56.397 | 80.314 | 1.00 | 16.85 |
| ATOM | 4190 | CE1 | PHE | A | 526 | 34.687 | 55.604 | 78.378 | 1.00 | 21.64 |
| ATOM | 4191 | CE2 | PHE | A | 526 | 33.698 | 55.298 | 80.567 | 1.00 | 19.90 |
| ATOM | 4192 | CZ  | PHE | A | 526 | 34.590 | 54.890 | 79.575 | 1.00 | 18.31 |
| ATOM | 4193 | N   | ASN | A | 527 | 31.418 | 61.433 | 77.949 | 1.00 | 12.75 |
| ATOM | 4194 | CA  | ASN | A | 527 | 30.391 | 62.355 | 77.446 | 1.00 | 12.28 |
| ATOM | 4195 | C   | ASN | A | 527 | 30.627 | 62.668 | 75.971 | 1.00 | 19.85 |
| ATOM | 4196 | O   | ASN | A | 527 | 29.715 | 62.907 | 75.185 | 1.00 | 18.13 |
| ATOM | 4197 | CB  | ASN | A | 527 | 30.431 | 63.713 | 78.160 | 1.00 | 13.86 |
| ATOM | 4198 | CG  | ASN | A | 527 | 29.641 | 63.696 | 79.434 | 1.00 | 25.14 |
| ATOM | 4199 | OD1 | ASN | A | 527 | 29.760 | 64.600 | 80.250 | 1.00 | 20.32 |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 4200 | ND2 | ASN | A | 527 | 28.830 | 62.668 | 79.610 | 1.00 | 10.82 |
| ATOM | 4201 | N   | ALA | A | 528 | 31.906 | 62.668 | 75.607 | 1.00 | 15.34 |
| ATOM | 4202 | CA  | ALA | A | 528 | 32.280 | 62.964 | 74.264 | 1.00 | 17.72 |
| ATOM | 4203 | C   | ALA | A | 528 | 32.075 | 61.861 | 73.228 | 1.00 | 26.48 |
| ATOM | 4204 | O   | ALA | A | 528 | 32.198 | 62.127 | 72.031 | 1.00 | 21.26 |
| ATOM | 4205 | CB  | ALA | A | 528 | 33.729 | 63.372 | 74.236 | 1.00 | 18.38 |
| ATOM | 4206 | N   | ILE | A | 529 | 31.810 | 60.629 | 73.664 | 1.00 | 19.00 |
| ATOM | 4207 | CA  | ILE | A | 529 | 31.690 | 59.524 | 72.731 | 1.00 | 15.58 |
| ATOM | 4208 | C   | ILE | A | 529 | 30.389 | 59.499 | 71.945 | 1.00 | 15.90 |
| ATOM | 4209 | O   | ILE | A | 529 | 29.305 | 59.561 | 72.494 | 1.00 | 16.45 |
| ATOM | 4210 | CB  | ILE | A | 529 | 31.946 | 58.208 | 73.454 | 1.00 | 17.38 |
| ATOM | 4211 | CG1 | ILE | A | 529 | 33.456 | 58.159 | 73.709 | 1.00 | 19.42 |
| ATOM | 4212 | CG2 | ILE | A | 529 | 31.511 | 57.103 | 72.488 | 1.00 | 17.67 |
| ATOM | 4213 | CD1 | ILE | A | 529 | 34.027 | 57.047 | 74.576 | 1.00 | 23.37 |
| ATOM | 4214 | N   | ASN | A | 530 | 30.440 | 59.418 | 70.641 | 1.00 | 16.94 |
| ATOM | 4215 | CA  | ASN | A | 530 | 29.151 | 59.417 | 69.969 | 1.00 | 20.74 |
| ATOM | 4216 | C   | ASN | A | 530 | 28.522 | 58.081 | 69.611 | 1.00 | 25.19 |
| ATOM | 4217 | O   | ASN | A | 530 | 27.369 | 58.026 | 69.217 | 1.00 | 23.63 |
| ATOM | 4218 | CB  | ASN | A | 530 | 28.937 | 60.566 | 68.986 | 1.00 | 39.14 |
| ATOM | 4219 | CG  | ASN | A | 530 | 28.612 | 61.852 | 69.749 | 1.00 | 80.92 |
| ATOM | 4220 | OD1 | ASN | A | 530 | 27.639 | 61.959 | 70.533 | 1.00 | 86.83 |
| ATOM | 4221 | ND2 | ASN | A | 530 | 29.470 | 62.838 | 69.537 | 1.00 | 45.14 |
| ATOM | 4222 | N   | ASN | A | 531 | 29.306 | 57.019 | 69.759 | 1.00 | 19.99 |
| ATOM | 4223 | CA  | ASN | A | 531 | 28.875 | 55.667 | 69.494 | 1.00 | 18.88 |
| ATOM | 4224 | C   | ASN | A | 531 | 27.637 | 55.452 | 70.350 | 1.00 | 15.67 |
| ATOM | 4225 | O   | ASN | A | 531 | 27.671 | 55.661 | 71.566 | 1.00 | 15.13 |
| ATOM | 4226 | CB  | ASN | A | 531 | 30.045 | 54.762 | 69.928 | 1.00 | 11.62 |
| ATOM | 4227 | CG  | ASN | A | 531 | 29.705 | 53.292 | 69.866 | 1.00 | 26.73 |
| ATOM | 4228 | OD1 | ASN | A | 531 | 28.724 | 52.832 | 70.471 | 1.00 | 21.97 |
| ATOM | 4229 | ND2 | ASN | A | 531 | 30.510 | 52.554 | 69.105 | 1.00 | 18.28 |
| ATOM | 4230 | N   | SER | A | 532 | 26.551 | 55.074 | 69.715 | 1.00 | 12.93 |
| ATOM | 4231 | CA  | SER | A | 532 | 25.293 | 54.931 | 70.456 | 1.00 | 15.99 |
| ATOM | 4232 | C   | SER | A | 532 | 25.248 | 53.889 | 71.565 | 1.00 | 17.50 |
| ATOM | 4233 | O   | SER | A | 532 | 24.631 | 54.066 | 72.611 | 1.00 | 20.47 |
| ATOM | 4234 | CB  | SER | A | 532 | 24.088 | 54.846 | 69.518 | 1.00 | 17.43 |
| ATOM | 4235 | OG  | SER | A | 532 | 24.274 | 53.791 | 68.570 | 1.00 | 24.83 |
| ATOM | 4236 | N   | GLU | A | 533 | 25.876 | 52.753 | 71.337 | 1.00 | 14.65 |
| ATOM | 4237 | CA  | GLU | A | 533 | 25.835 | 51.708 | 72.339 | 1.00 | 13.13 |
| ATOM | 4238 | C   | GLU | A | 533 | 26.497 | 52.181 | 73.614 | 1.00 | 19.42 |
| ATOM | 4239 | O   | GLU | A | 533 | 25.964 | 52.028 | 74.725 | 1.00 | 15.25 |
| ATOM | 4240 | CB  | GLU | A | 533 | 26.547 | 50.464 | 71.780 | 1.00 | 13.22 |
| ATOM | 4241 | CG  | GLU | A | 533 | 25.712 | 49.829 | 70.637 | 1.00 | 9.87  |
| ATOM | 4242 | CD  | GLU | A | 533 | 24.531 | 49.055 | 71.162 | 1.00 | 21.99 |
| ATOM | 4243 | OE1 | GLU | A | 533 | 24.395 | 48.722 | 72.319 | 1.00 | 18.49 |
| ATOM | 4244 | OE2 | GLU | A | 533 | 23.625 | 48.805 | 70.267 | 1.00 | 16.24 |
| ATOM | 4245 | N   | ILE | A | 534 | 27.686 | 52.747 | 73.415 | 1.00 | 15.22 |
| ATOM | 4246 | CA  | ILE | A | 534 | 28.495 | 53.265 | 74.512 | 1.00 | 14.94 |
| ATOM | 4247 | C   | ILE | A | 534 | 27.793 | 54.420 | 75.228 | 1.00 | 14.04 |
| ATOM | 4248 | O   | ILE | A | 534 | 27.677 | 54.447 | 76.461 | 1.00 | 17.42 |
| ATOM | 4249 | CB  | ILE | A | 534 | 29.926 | 53.655 | 74.077 | 1.00 | 17.98 |
| ATOM | 4250 | CG1 | ILE | A | 534 | 30.733 | 52.461 | 73.557 | 1.00 | 13.41 |
| ATOM | 4251 | CG2 | ILE | A | 534 | 30.680 | 54.387 | 75.216 | 1.00 | 15.34 |
| ATOM | 4252 | CD1 | ILE | A | 534 | 32.003 | 52.906 | 72.825 | 1.00 | 17.39 |
| ATOM | 4253 | N   | ARG | A | 535 | 27.310 | 55.402 | 74.475 | 1.00 | 14.39 |
| ATOM | 4254 | CA  | ARG | A | 535 | 26.611 | 56.511 | 75.135 | 1.00 | 17.35 |
| ATOM | 4255 | C   | ARG | A | 535 | 25.347 | 56.016 | 75.868 | 1.00 | 14.54 |
| ATOM | 4256 | O   | ARG | A | 535 | 24.998 | 56.382 | 76.973 | 1.00 | 15.05 |
| ATOM | 4257 | CB  | ARG | A | 535 | 26.232 | 57.576 | 74.108 | 1.00 | 16.26 |
| ATOM | 4258 | CG  | ARG | A | 535 | 25.583 | 58.826 | 74.730 | 1.00 | 8.73  |
| ATOM | 4259 | CD  | ARG | A | 535 | 25.392 | 59.919 | 73.666 | 1.00 | 11.55 |
| ATOM | 4260 | NE  | ARG | A | 535 | 25.126 | 61.228 | 74.251 | 1.00 | 15.18 |



0012340-003600

|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 4261 | CZ  | ARG | A | 535 | 26.049 | 62.043 | 74.761 | 1.00 | 26.20 |
| ATOM | 4262 | NH1 | ARG | A | 535 | 27.354 | 61.765 | 74.769 | 1.00 | 20.26 |
| ATOM | 4263 | NH2 | ARG | A | 535 | 25.636 | 63.189 | 75.286 | 1.00 | 19.91 |
| ATOM | 4264 | N   | PHE | A | 536 | 24.632 | 55.126 | 75.233 | 1.00 | 11.71 |
| ATOM | 4265 | CA  | PHE | A | 536 | 23.462 | 54.627 | 75.876 | 1.00 | 9.63  |
| ATOM | 4266 | C   | PHE | A | 536 | 23.825 | 54.092 | 77.233 | 1.00 | 13.77 |
| ATOM | 4267 | O   | PHE | A | 536 | 23.256 | 54.497 | 78.231 | 1.00 | 13.81 |
| ATOM | 4268 | CB  | PHE | A | 536 | 22.906 | 53.471 | 75.016 | 1.00 | 10.66 |
| ATOM | 4269 | CG  | PHE | A | 536 | 21.865 | 52.621 | 75.710 | 1.00 | 14.64 |
| ATOM | 4270 | CD1 | PHE | A | 536 | 20.699 | 53.158 | 76.256 | 1.00 | 13.81 |
| ATOM | 4271 | CD2 | PHE | A | 536 | 22.052 | 51.242 | 75.840 | 1.00 | 19.23 |
| ATOM | 4272 | CE1 | PHE | A | 536 | 19.762 | 52.325 | 76.877 | 1.00 | 14.23 |
| ATOM | 4273 | CE2 | PHE | A | 536 | 21.127 | 50.395 | 76.457 | 1.00 | 16.53 |
| ATOM | 4274 | CZ  | PHE | A | 536 | 19.960 | 50.945 | 76.984 | 1.00 | 11.63 |
| ATOM | 4275 | N   | ARG | A | 537 | 24.750 | 53.131 | 77.282 | 1.00 | 12.89 |
| ATOM | 4276 | CA  | ARG | A | 537 | 25.110 | 52.536 | 78.577 | 1.00 | 11.92 |
| ATOM | 4277 | C   | ARG | A | 537 | 25.734 | 53.520 | 79.575 | 1.00 | 16.03 |
| ATOM | 4278 | O   | ARG | A | 537 | 25.525 | 53.436 | 80.793 | 1.00 | 10.71 |
| ATOM | 4279 | CB  | ARG | A | 537 | 25.949 | 51.253 | 78.505 | 1.00 | 11.85 |
| ATOM | 4280 | CG  | ARG | A | 537 | 25.274 | 50.113 | 77.776 | 1.00 | 8.59  |
| ATOM | 4281 | CD  | ARG | A | 537 | 26.142 | 48.857 | 77.547 | 1.00 | 17.16 |
| ATOM | 4282 | NE  | ARG | A | 537 | 25.233 | 47.845 | 76.992 | 1.00 | 16.12 |
| ATOM | 4283 | CZ  | ARG | A | 537 | 24.869 | 47.824 | 75.716 | 1.00 | 25.23 |
| ATOM | 4284 | NH1 | ARG | A | 537 | 25.414 | 48.641 | 74.802 | 1.00 | 13.55 |
| ATOM | 4285 | NH2 | ARG | A | 537 | 23.946 | 46.947 | 75.356 | 1.00 | 16.52 |
| ATOM | 4286 | N   | TRP | A | 538 | 26.544 | 54.451 | 79.060 | 1.00 | 13.16 |
| ATOM | 4287 | CA  | TRP | A | 538 | 27.170 | 55.440 | 79.907 | 1.00 | 10.77 |
| ATOM | 4288 | C   | TRP | A | 538 | 26.079 | 56.286 | 80.532 | 1.00 | 13.43 |
| ATOM | 4289 | O   | TRP | A | 538 | 26.048 | 56.509 | 81.736 | 1.00 | 13.45 |
| ATOM | 4290 | CB  | TRP | A | 538 | 28.036 | 56.318 | 78.996 | 1.00 | 12.97 |
| ATOM | 4291 | CG  | TRP | A | 538 | 28.489 | 57.611 | 79.604 | 1.00 | 12.46 |
| ATOM | 4292 | CD1 | TRP | A | 538 | 28.330 | 58.807 | 79.019 | 1.00 | 13.56 |
| ATOM | 4293 | CD2 | TRP | A | 538 | 29.199 | 57.826 | 80.857 | 1.00 | 11.95 |
| ATOM | 4294 | NE1 | TRP | A | 538 | 28.932 | 59.757 | 79.801 | 1.00 | 12.84 |
| ATOM | 4295 | CE2 | TRP | A | 538 | 29.455 | 59.208 | 80.938 | 1.00 | 12.68 |
| ATOM | 4296 | CE3 | TRP | A | 538 | 29.667 | 57.000 | 81.914 | 1.00 | 11.87 |
| ATOM | 4297 | CZ2 | TRP | A | 538 | 30.115 | 59.780 | 82.024 | 1.00 | 10.55 |
| ATOM | 4298 | CZ3 | TRP | A | 538 | 30.334 | 57.557 | 82.994 | 1.00 | 12.97 |
| ATOM | 4299 | CH2 | TRP | A | 538 | 30.537 | 58.953 | 83.046 | 1.00 | 14.62 |
| ATOM | 4300 | N   | LEU | A | 539 | 25.160 | 56.761 | 79.714 | 1.00 | 8.88  |
| ATOM | 4301 | CA  | LEU | A | 539 | 24.132 | 57.592 | 80.310 | 1.00 | 11.52 |
| ATOM | 4302 | C   | LEU | A | 539 | 23.249 | 56.878 | 81.335 | 1.00 | 17.64 |
| ATOM | 4303 | O   | LEU | A | 539 | 22.775 | 57.470 | 82.308 | 1.00 | 15.29 |
| ATOM | 4304 | CB  | LEU | A | 539 | 23.253 | 58.271 | 79.251 | 1.00 | 13.68 |
| ATOM | 4305 | CG  | LEU | A | 539 | 23.977 | 59.247 | 78.323 | 1.00 | 15.24 |
| ATOM | 4306 | CD1 | LEU | A | 539 | 22.989 | 59.923 | 77.388 | 1.00 | 13.27 |
| ATOM | 4307 | CD2 | LEU | A | 539 | 24.693 | 60.312 | 79.121 | 1.00 | 13.80 |
| ATOM | 4308 | N   | ARG | A | 540 | 22.988 | 55.583 | 81.115 | 1.00 | 14.05 |
| ATOM | 4309 | CA  | ARG | A | 540 | 22.176 | 54.850 | 82.067 | 1.00 | 11.62 |
| ATOM | 4310 | C   | ARG | A | 540 | 22.880 | 54.792 | 83.418 | 1.00 | 13.27 |
| ATOM | 4311 | O   | ARG | A | 540 | 22.277 | 54.942 | 84.488 | 1.00 | 12.86 |
| ATOM | 4312 | CB  | ARG | A | 540 | 21.883 | 53.426 | 81.584 | 1.00 | 12.88 |
| ATOM | 4313 | CG  | ARG | A | 540 | 20.894 | 53.325 | 80.408 | 1.00 | 8.76  |
| ATOM | 4314 | CD  | ARG | A | 540 | 20.453 | 51.857 | 80.281 | 1.00 | 14.08 |
| ATOM | 4315 | NE  | ARG | A | 540 | 19.442 | 51.552 | 81.288 | 1.00 | 11.93 |
| ATOM | 4316 | CZ  | ARG | A | 540 | 18.856 | 50.391 | 81.486 | 1.00 | 16.72 |
| ATOM | 4317 | NH1 | ARG | A | 540 | 19.145 | 49.317 | 80.774 | 1.00 | 16.31 |
| ATOM | 4318 | NH2 | ARG | A | 540 | 17.926 | 50.330 | 82.416 | 1.00 | 9.86  |
| ATOM | 4319 | N   | LEU | A | 541 | 24.189 | 54.546 | 83.338 | 1.00 | 10.69 |
| ATOM | 4320 | CA  | LEU | A | 541 | 25.036 | 54.432 | 84.526 | 1.00 | 9.89  |
| ATOM | 4321 | C   | LEU | A | 541 | 25.017 | 55.712 | 85.353 | 1.00 | 12.38 |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 4322 | O   | LEU | A | 541 | 24.961 | 55.749 | 86.598 | 1.00 | 12.85 |
| ATOM | 4323 | CB  | LEU | A | 541 | 26.482 | 54.119 | 84.074 | 1.00 | 8.98  |
| ATOM | 4324 | CG  | LEU | A | 541 | 27.519 | 53.986 | 85.194 | 1.00 | 13.06 |
| ATOM | 4325 | CD1 | LEU | A | 541 | 27.144 | 52.889 | 86.196 | 1.00 | 11.30 |
| ATOM | 4326 | CD2 | LEU | A | 541 | 28.904 | 53.697 | 84.606 | 1.00 | 11.15 |
| ATOM | 4327 | N   | CYS | A | 542 | 25.097 | 56.800 | 84.603 | 1.00 | 14.91 |
| ATOM | 4328 | CA  | CYS | A | 542 | 25.043 | 58.147 | 85.153 | 1.00 | 15.42 |
| ATOM | 4329 | C   | CYS | A | 542 | 23.719 | 58.436 | 85.881 | 1.00 | 12.87 |
| ATOM | 4330 | O   | CYS | A | 542 | 23.689 | 58.913 | 87.019 | 1.00 | 13.42 |
| ATOM | 4331 | CB  | CYS | A | 542 | 25.234 | 59.166 | 83.987 | 1.00 | 14.29 |
| ATOM | 4332 | SG  | CYS | A | 542 | 26.987 | 59.258 | 83.516 | 1.00 | 15.48 |
| ATOM | 4333 | N   | ILE | A | 543 | 22.620 | 58.161 | 85.188 | 1.00 | 11.12 |
| ATOM | 4334 | CA  | ILE | A | 543 | 21.287 | 58.388 | 85.723 | 1.00 | 12.92 |
| ATOM | 4335 | C   | ILE | A | 543 | 21.034 | 57.514 | 86.912 | 1.00 | 15.64 |
| ATOM | 4336 | O   | ILE | A | 543 | 20.565 | 57.959 | 87.965 | 1.00 | 14.40 |
| ATOM | 4337 | CB  | ILE | A | 543 | 20.193 | 58.168 | 84.670 | 1.00 | 14.69 |
| ATOM | 4338 | CG1 | ILE | A | 543 | 20.350 | 59.208 | 83.580 | 1.00 | 14.31 |
| ATOM | 4339 | CG2 | ILE | A | 543 | 18.785 | 58.292 | 85.281 | 1.00 | 11.05 |
| ATOM | 4340 | CD1 | ILE | A | 543 | 20.139 | 60.651 | 84.095 | 1.00 | 13.56 |
| ATOM | 4341 | N   | GLN | A | 544 | 21.362 | 56.237 | 86.729 | 1.00 | 13.09 |
| ATOM | 4342 | CA  | GLN | A | 544 | 21.144 | 55.310 | 87.829 | 1.00 | 12.90 |
| ATOM | 4343 | C   | GLN | A | 544 | 22.017 | 55.629 | 89.015 | 1.00 | 16.30 |
| ATOM | 4344 | O   | GLN | A | 544 | 21.649 | 55.299 | 90.140 | 1.00 | 12.81 |
| ATOM | 4345 | CB  | GLN | A | 544 | 21.287 | 53.846 | 87.396 | 1.00 | 14.77 |
| ATOM | 4346 | CG  | GLN | A | 544 | 20.159 | 53.374 | 86.449 | 1.00 | 13.43 |
| ATOM | 4347 | CD  | GLN | A | 544 | 20.399 | 51.967 | 85.889 | 1.00 | 16.60 |
| ATOM | 4348 | OE1 | GLN | A | 544 | 20.048 | 51.639 | 84.754 | 1.00 | 18.63 |
| ATOM | 4349 | NE2 | GLN | A | 544 | 20.976 | 51.100 | 86.695 | 1.00 | 7.00  |
| ATOM | 4350 | N   | SER | A | 545 | 23.143 | 56.296 | 88.748 | 1.00 | 13.80 |
| ATOM | 4351 | CA  | SER | A | 545 | 24.058 | 56.712 | 89.799 | 1.00 | 13.01 |
| ATOM | 4352 | C   | SER | A | 545 | 23.715 | 58.091 | 90.368 | 1.00 | 17.51 |
| ATOM | 4353 | O   | SER | A | 545 | 24.429 | 58.656 | 91.189 | 1.00 | 17.76 |
| ATOM | 4354 | CB  | SER | A | 545 | 25.495 | 56.649 | 89.330 | 1.00 | 14.26 |
| ATOM | 4355 | OG  | SER | A | 545 | 25.735 | 55.273 | 89.138 | 1.00 | 15.74 |
| ATOM | 4356 | N   | LYS | A | 546 | 22.586 | 58.609 | 89.924 | 1.00 | 13.25 |
| ATOM | 4357 | CA  | LYS | A | 546 | 22.029 | 59.857 | 90.370 | 1.00 | 14.37 |
| ATOM | 4358 | C   | LYS | A | 546 | 22.771 | 61.109 | 89.963 | 1.00 | 16.71 |
| ATOM | 4359 | O   | LYS | A | 546 | 22.770 | 62.106 | 90.698 | 1.00 | 16.30 |
| ATOM | 4360 | CB  | LYS | A | 546 | 21.850 | 59.890 | 91.878 | 1.00 | 15.93 |
| ATOM | 4361 | CG  | LYS | A | 546 | 21.320 | 58.602 | 92.470 | 1.00 | 16.80 |
| ATOM | 4362 | CD  | LYS | A | 546 | 19.919 | 58.370 | 91.982 | 1.00 | 13.30 |
| ATOM | 4363 | CE  | LYS | A | 546 | 19.280 | 57.148 | 92.617 | 1.00 | 24.82 |
| ATOM | 4364 | NZ  | LYS | A | 546 | 18.052 | 56.742 | 91.905 | 1.00 | 17.92 |
| ATOM | 4365 | N   | TRP | A | 547 | 23.418 | 61.104 | 88.827 | 1.00 | 15.72 |
| ATOM | 4366 | CA  | TRP | A | 547 | 24.103 | 62.319 | 88.438 | 1.00 | 16.24 |
| ATOM | 4367 | C   | TRP | A | 547 | 23.132 | 63.246 | 87.727 | 1.00 | 18.78 |
| ATOM | 4368 | O   | TRP | A | 547 | 22.760 | 63.007 | 86.605 | 1.00 | 16.35 |
| ATOM | 4369 | CB  | TRP | A | 547 | 25.261 | 61.999 | 87.505 | 1.00 | 15.42 |
| ATOM | 4370 | CG  | TRP | A | 547 | 26.211 | 63.156 | 87.344 | 1.00 | 16.84 |
| ATOM | 4371 | CD1 | TRP | A | 547 | 26.177 | 64.386 | 87.949 | 1.00 | 18.62 |
| ATOM | 4372 | CD2 | TRP | A | 547 | 27.349 | 63.140 | 86.479 | 1.00 | 15.94 |
| ATOM | 4373 | NE1 | TRP | A | 547 | 27.267 | 65.115 | 87.543 | 1.00 | 16.22 |
| ATOM | 4374 | CE2 | TRP | A | 547 | 27.997 | 64.380 | 86.629 | 1.00 | 18.06 |
| ATOM | 4375 | CE3 | TRP | A | 547 | 27.900 | 62.159 | 85.647 | 1.00 | 16.57 |
| ATOM | 4376 | CZ2 | TRP | A | 547 | 29.186 | 64.662 | 85.928 | 1.00 | 16.68 |
| ATOM | 4377 | CZ3 | TRP | A | 547 | 29.068 | 62.459 | 84.966 | 1.00 | 19.03 |
| ATOM | 4378 | CH2 | TRP | A | 547 | 29.693 | 63.709 | 85.079 | 1.00 | 18.04 |
| ATOM | 4379 | N   | GLU | A | 548 | 22.706 | 64.327 | 88.376 | 1.00 | 13.95 |
| ATOM | 4380 | CA  | GLU | A | 548 | 21.745 | 65.238 | 87.780 | 1.00 | 13.21 |
| ATOM | 4381 | C   | GLU | A | 548 | 22.176 | 65.856 | 86.468 | 1.00 | 17.27 |
| ATOM | 4382 | O   | GLU | A | 548 | 21.352 | 66.149 | 85.617 | 1.00 | 18.18 |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 4383 | CB  | GLU | A | 548 | 21.375 | 66.370 | 88.771 | 1.00 | 15.29 |
| ATOM | 4384 | CG  | GLU | A | 548 | 20.751 | 65.878 | 90.109 | 1.00 | 19.42 |
| ATOM | 4385 | CD  | GLU | A | 548 | 20.207 | 67.018 | 90.953 | 1.00 | 33.00 |
| ATOM | 4386 | OE1 | GLU | A | 548 | 19.775 | 68.057 | 90.492 | 1.00 | 46.88 |
| ATOM | 4387 | OE2 | GLU | A | 548 | 20.224 | 66.791 | 92.239 | 1.00 | 30.89 |
| ATOM | 4388 | N   | ASP | A | 549 | 23.477 | 66.105 | 86.285 | 1.00 | 17.99 |
| ATOM | 4389 | CA  | ASP | A | 549 | 23.929 | 66.735 | 85.054 | 1.00 | 10.58 |
| ATOM | 4390 | C   | ASP | A | 549 | 23.666 | 65.896 | 83.853 | 1.00 | 12.02 |
| ATOM | 4391 | O   | ASP | A | 549 | 23.629 | 66.354 | 82.709 | 1.00 | 18.87 |
| ATOM | 4392 | CB  | ASP | A | 549 | 25.426 | 67.034 | 85.126 | 1.00 | 11.36 |
| ATOM | 4393 | CG  | ASP | A | 549 | 25.703 | 68.058 | 86.214 | 1.00 | 22.44 |
| ATOM | 4394 | OD1 | ASP | A | 549 | 25.396 | 69.227 | 86.150 | 1.00 | 25.44 |
| ATOM | 4395 | OD2 | ASP | A | 549 | 26.252 | 67.575 | 87.271 | 1.00 | 25.86 |
| ATOM | 4396 | N   | ALA | A | 550 | 23.511 | 64.624 | 84.122 | 1.00 | 13.24 |
| ATOM | 4397 | CA  | ALA | A | 550 | 23.269 | 63.709 | 83.004 | 1.00 | 14.70 |
| ATOM | 4398 | C   | ALA | A | 550 | 21.845 | 63.707 | 82.473 | 1.00 | 17.89 |
| ATOM | 4399 | O   | ALA | A | 550 | 21.598 | 63.132 | 81.389 | 1.00 | 15.28 |
| ATOM | 4400 | CB  | ALA | A | 550 | 23.713 | 62.280 | 83.335 | 1.00 | 14.77 |
| ATOM | 4401 | N   | ILE | A | 551 | 20.926 | 64.308 | 83.251 | 1.00 | 16.18 |
| ATOM | 4402 | CA  | ILE | A | 551 | 19.497 | 64.377 | 82.914 | 1.00 | 16.05 |
| ATOM | 4403 | C   | ILE | A | 551 | 19.182 | 64.894 | 81.523 | 1.00 | 18.70 |
| ATOM | 4404 | O   | ILE | A | 551 | 18.441 | 64.290 | 80.736 | 1.00 | 19.01 |
| ATOM | 4405 | CB  | ILE | A | 551 | 18.701 | 65.139 | 83.971 | 1.00 | 19.52 |
| ATOM | 4406 | CG1 | ILE | A | 551 | 18.692 | 64.281 | 85.232 | 1.00 | 20.39 |
| ATOM | 4407 | CG2 | ILE | A | 551 | 17.251 | 65.361 | 83.512 | 1.00 | 12.65 |
| ATOM | 4408 | CD1 | ILE | A | 551 | 18.167 | 64.995 | 86.485 | 1.00 | 15.78 |
| ATOM | 4409 | N   | PRO | A | 552 | 19.748 | 66.038 | 81.197 | 1.00 | 18.48 |
| ATOM | 4410 | CA  | PRO | A | 552 | 19.487 | 66.600 | 79.888 | 1.00 | 16.36 |
| ATOM | 4411 | C   | PRO | A | 552 | 20.084 | 65.736 | 78.795 | 1.00 | 19.64 |
| ATOM | 4412 | O   | PRO | A | 552 | 19.551 | 65.606 | 77.700 | 1.00 | 16.94 |
| ATOM | 4413 | CB  | PRO | A | 552 | 20.125 | 67.995 | 79.870 | 1.00 | 18.41 |
| ATOM | 4414 | CG  | PRO | A | 552 | 21.001 | 68.070 | 81.116 | 1.00 | 24.69 |
| ATOM | 4415 | CD  | PRO | A | 552 | 20.504 | 66.981 | 82.059 | 1.00 | 17.97 |
| ATOM | 4416 | N   | LEU | A | 553 | 21.226 | 65.144 | 79.075 | 1.00 | 17.67 |
| ATOM | 4417 | CA  | LEU | A | 553 | 21.852 | 64.302 | 78.072 | 1.00 | 15.47 |
| ATOM | 4418 | C   | LEU | A | 553 | 20.940 | 63.101 | 77.795 | 1.00 | 19.23 |
| ATOM | 4419 | O   | LEU | A | 553 | 20.704 | 62.655 | 76.681 | 1.00 | 16.64 |
| ATOM | 4420 | CB  | LEU | A | 553 | 23.275 | 63.819 | 78.501 | 1.00 | 13.81 |
| ATOM | 4421 | CG  | LEU | A | 553 | 24.239 | 64.905 | 79.002 | 1.00 | 19.25 |
| ATOM | 4422 | CD1 | LEU | A | 553 | 25.606 | 64.289 | 79.247 | 1.00 | 17.04 |
| ATOM | 4423 | CD2 | LEU | A | 553 | 24.412 | 65.997 | 77.955 | 1.00 | 18.39 |
| ATOM | 4424 | N   | ALA | A | 554 | 20.440 | 62.529 | 78.867 | 1.00 | 17.65 |
| ATOM | 4425 | CA  | ALA | A | 554 | 19.614 | 6      |        |      |       |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 4444 | CE  | LYS | A | 556 | 21.851 | 66.449 | 71.883 | 1.00 | 79.74 |
| ATOM | 4445 | NZ  | LYS | A | 556 | 22.446 | 67.709 | 71.404 | 1.00 | 60.52 |
| ATOM | 4446 | N   | MET | A | 557 | 19.089 | 62.128 | 74.207 | 1.00 | 15.27 |
| ATOM | 4447 | CA  | MET | A | 557 | 19.294 | 60.904 | 73.446 | 1.00 | 13.47 |
| ATOM | 4448 | C   | MET | A | 557 | 17.997 | 60.140 | 73.264 | 1.00 | 16.45 |
| ATOM | 4449 | O   | MET | A | 557 | 17.723 | 59.507 | 72.253 | 1.00 | 15.63 |
| ATOM | 4450 | CB  | MET | A | 557 | 20.312 | 59.998 | 74.165 | 1.00 | 14.26 |
| ATOM | 4451 | CG  | MET | A | 557 | 20.499 | 58.682 | 73.405 | 1.00 | 13.00 |
| ATOM | 4452 | SD  | MET | A | 557 | 21.984 | 57.796 | 73.915 | 1.00 | 16.44 |
| ATOM | 4453 | CE  | MET | A | 557 | 22.027 | 56.574 | 72.596 | 1.00 | 12.39 |
| ATOM | 4454 | N   | ALA | A | 558 | 17.200 | 60.181 | 74.327 | 1.00 | 18.08 |
| ATOM | 4455 | CA  | ALA | A | 558 | 15.955 | 59.438 | 74.323 | 1.00 | 17.49 |
| ATOM | 4456 | C   | ALA | A | 558 | 14.968 | 59.922 | 73.292 | 1.00 | 23.08 |
| ATOM | 4457 | O   | ALA | A | 558 | 14.221 | 59.153 | 72.723 | 1.00 | 21.14 |
| ATOM | 4458 | CB  | ALA | A | 558 | 15.316 | 59.439 | 75.705 | 1.00 | 16.55 |
| ATOM | 4459 | N   | THR | A | 559 | 14.951 | 61.220 | 73.082 | 1.00 | 18.89 |
| ATOM | 4460 | CA  | THR | A | 559 | 13.980 | 61.798 | 72.186 | 1.00 | 19.50 |
| ATOM | 4461 | C   | THR | A | 559 | 14.542 | 62.125 | 70.830 | 1.00 | 22.12 |
| ATOM | 4462 | O   | THR | A | 559 | 13.804 | 62.219 | 69.862 | 1.00 | 23.28 |
| ATOM | 4463 | CB  | THR | A | 559 | 13.418 | 63.078 | 72.824 | 1.00 | 25.23 |
| ATOM | 4464 | OG1 | THR | A | 559 | 14.493 | 63.999 | 73.001 | 1.00 | 22.20 |
| ATOM | 4465 | CG2 | THR | A | 559 | 12.734 | 62.723 | 74.147 | 1.00 | 18.19 |
| ATOM | 4466 | N   | GLU | A | 560 | 15.841 | 62.316 | 70.756 | 1.00 | 16.68 |
| ATOM | 4467 | CA  | GLU | A | 560 | 16.399 | 62.646 | 69.479 | 1.00 | 18.60 |
| ATOM | 4468 | C   | GLU | A | 560 | 16.492 | 61.448 | 68.545 | 1.00 | 26.45 |
| ATOM | 4469 | O   | GLU | A | 560 | 16.714 | 61.608 | 67.344 | 1.00 | 21.93 |
| ATOM | 4470 | CB  | GLU | A | 560 | 17.748 | 63.317 | 69.640 | 1.00 | 21.55 |
| ATOM | 4471 | CG  | GLU | A | 560 | 17.623 | 64.757 | 70.136 | 1.00 | 38.31 |
| ATOM | 4472 | CD  | GLU | A | 560 | 18.990 | 65.352 | 70.221 | 1.00 | 55.37 |
| ATOM | 4473 | OE1 | GLU | A | 560 | 20.007 | 64.691 | 70.053 | 1.00 | 40.21 |
| ATOM | 4474 | OE2 | GLU | A | 560 | 18.946 | 66.627 | 70.504 | 1.00 | 55.04 |
| ATOM | 4475 | N   | GLN | A | 561 | 16.344 | 60.251 | 69.101 | 1.00 | 20.47 |
| ATOM | 4476 | CA  | GLN | A | 561 | 16.340 | 59.043 | 68.291 | 1.00 | 19.24 |
| ATOM | 4477 | C   | GLN | A | 561 | 15.283 | 58.189 | 68.921 | 1.00 | 18.06 |
| ATOM | 4478 | O   | GLN | A | 561 | 14.874 | 58.520 | 70.022 | 1.00 | 16.87 |
| ATOM | 4479 | CB  | GLN | A | 561 | 17.684 | 58.307 | 68.136 | 1.00 | 20.45 |
| ATOM | 4480 | CG  | GLN | A | 561 | 18.341 | 58.001 | 69.495 | 1.00 | 21.17 |
| ATOM | 4481 | CD  | GLN | A | 561 | 17.692 | 56.815 | 70.165 | 1.00 | 21.31 |
| ATOM | 4482 | OE1 | GLN | A | 561 | 17.302 | 56.877 | 71.344 | 1.00 | 23.07 |
| ATOM | 4483 | NE2 | GLN | A | 561 | 17.543 | 55.758 | 69.379 | 1.00 | 11.21 |
| ATOM | 4484 | N   | GLY | A | 562 | 14.821 | 57.148 | 68.239 | 1.00 | 16.15 |
| ATOM | 4485 | CA  | GLY | A | 562 | 13.758 | 56.367 | 68.827 | 1.00 | 14.79 |
| ATOM | 4486 | C   | GLY | A | 562 | 13.919 |        |        |      |       |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 4505 | SD  | MET | A | 564 | 9.692  | 49.805 | 70.530 | 1.00 | 21.23 |
| ATOM | 4506 | CE  | MET | A | 564 | 10.114 | 48.581 | 69.265 | 1.00 | 17.64 |
| ATOM | 4507 | N   | LYS | A | 565 | 15.464 | 50.097 | 71.892 | 1.00 | 16.37 |
| ATOM | 4508 | CA  | LYS | A | 565 | 16.521 | 49.537 | 72.701 | 1.00 | 13.75 |
| ATOM | 4509 | C   | LYS | A | 565 | 17.129 | 50.623 | 73.582 | 1.00 | 16.90 |
| ATOM | 4510 | O   | LYS | A | 565 | 17.493 | 50.376 | 74.735 | 1.00 | 14.97 |
| ATOM | 4511 | CB  | LYS | A | 565 | 17.549 | 48.885 | 71.767 | 1.00 | 11.37 |
| ATOM | 4512 | CG  | LYS | A | 565 | 18.793 | 48.371 | 72.459 | 1.00 | 12.72 |
| ATOM | 4513 | CD  | LYS | A | 565 | 19.962 | 48.100 | 71.525 | 1.00 | 17.72 |
| ATOM | 4514 | CE  | LYS | A | 565 | 21.060 | 47.336 | 72.239 | 1.00 | 19.39 |
| ATOM | 4515 | NZ  | LYS | A | 565 | 22.030 | 46.721 | 71.308 | 1.00 | 15.41 |
| ATOM | 4516 | N   | PHE | A | 566 | 17.211 | 51.847 | 73.057 | 1.00 | 12.01 |
| ATOM | 4517 | CA  | PHE | A | 566 | 17.801 | 52.912 | 73.846 | 1.00 | 12.25 |
| ATOM | 4518 | C   | PHE | A | 566 | 16.739 | 53.770 | 74.509 | 1.00 | 15.74 |
| ATOM | 4519 | O   | PHE | A | 566 | 16.843 | 54.177 | 75.661 | 1.00 | 12.91 |
| ATOM | 4520 | CB  | PHE | A | 566 | 18.641 | 53.814 | 72.932 | 1.00 | 12.87 |
| ATOM | 4521 | CG  | PHE | A | 566 | 19.744 | 53.117 | 72.165 | 1.00 | 14.44 |
| ATOM | 4522 | CD1 | PHE | A | 566 | 20.465 | 52.053 | 72.714 | 1.00 | 13.84 |
| ATOM | 4523 | CD2 | PHE | A | 566 | 20.111 | 53.577 | 70.894 | 1.00 | 15.31 |
| ATOM | 4524 | CE1 | PHE | A | 566 | 21.510 | 51.434 | 72.014 | 1.00 | 13.86 |
| ATOM | 4525 | CE2 | PHE | A | 566 | 21.145 | 52.977 | 70.172 | 1.00 | 14.39 |
| ATOM | 4526 | CZ  | PHE | A | 566 | 21.849 | 51.910 | 70.744 | 1.00 | 15.76 |
| ATOM | 4527 | N   | THR | A | 567 | 15.721 | 54.095 | 73.724 | 1.00 | 16.10 |
| ATOM | 4528 | CA  | THR | A | 567 | 14.642 | 54.966 | 74.184 | 1.00 | 14.70 |
| ATOM | 4529 | C   | THR | A | 567 | 13.876 | 54.518 | 75.423 | 1.00 | 14.32 |
| ATOM | 4530 | O   | THR | A | 567 | 13.615 | 55.315 | 76.346 | 1.00 | 14.88 |
| ATOM | 4531 | CB  | THR | A | 567 | 13.707 | 55.409 | 73.030 | 1.00 | 14.81 |
| ATOM | 4532 | OG1 | THR | A | 567 | 14.465 | 56.204 | 72.148 | 1.00 | 15.28 |
| ATOM | 4533 | CG2 | THR | A | 567 | 12.520 | 56.196 | 73.596 | 1.00 | 14.89 |
| ATOM | 4534 | N   | ARG | A | 568 | 13.478 | 53.245 | 75.412 | 1.00 | 12.20 |
| ATOM | 4535 | CA  | ARG | A | 568 | 12.697 | 52.764 | 76.533 | 1.00 | 13.57 |
| ATOM | 4536 | C   | ARG | A | 568 | 13.393 | 52.797 | 77.876 | 1.00 | 14.85 |
| ATOM | 4537 | O   | ARG | A | 568 | 12.896 | 53.312 | 78.861 | 1.00 | 14.39 |
| ATOM | 4538 | CB  | ARG | A | 568 | 12.133 | 51.400 | 76.218 | 1.00 | 13.49 |
| ATOM | 4539 | CG  | ARG | A | 568 | 11.021 | 51.467 | 75.155 | 1.00 | 14.02 |
| ATOM | 4540 | CD  | ARG | A | 568 | 10.387 | 50.098 | 74.884 | 1.00 | 9.84  |
| ATOM | 4541 | NE  | ARG | A | 568 | 9.662  | 49.607 | 76.063 | 1.00 | 13.61 |
| ATOM | 4542 | CZ  | ARG | A | 568 | 9.236  | 48.368 | 76.197 | 1.00 | 17.32 |
| ATOM | 4543 | NH1 | ARG | A | 568 | 9.471  | 47.427 | 75.275 | 1.00 | 13.23 |
| ATOM | 4544 | NH2 | ARG | A | 568 | 8.566  | 48.053 | 77.293 | 1.00 | 13.32 |
| ATOM | 4545 | N   | PRO | A | 569 | 14.577 | 52.237 | 77.948 | 1.00 | 12.95 |
| ATOM | 4546 | CA  | PRO | A | 569 | 15.294 | 52.206 | 79.229 | 1.00 | 10.82 |
| ATOM | 4547 | C   | PRO | A | 569 | 15.810 | 53.574 |        |      |       |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 4566 | CD1 | PHE | A | 571 | 11.035 | 59.194 | 78.591 | 1.00 | 18.00 |
| ATOM | 4567 | CD2 | PHE | A | 571 | 11.634 | 57.902 | 76.633 | 1.00 | 19.72 |
| ATOM | 4568 | CE1 | PHE | A | 571 | 10.768 | 60.317 | 77.805 | 1.00 | 17.86 |
| ATOM | 4569 | CE2 | PHE | A | 571 | 11.358 | 59.016 | 75.836 | 1.00 | 23.80 |
| ATOM | 4570 | CZ  | PHE | A | 571 | 10.933 | 60.213 | 76.422 | 1.00 | 22.47 |
| ATOM | 4571 | N   | LYS | A | 572 | 12.839 | 55.023 | 81.080 | 1.00 | 14.21 |
| ATOM | 4572 | CA  | LYS | A | 572 | 12.530 | 54.361 | 82.325 | 1.00 | 14.07 |
| ATOM | 4573 | C   | LYS | A | 572 | 13.476 | 54.788 | 83.444 | 1.00 | 16.22 |
| ATOM | 4574 | O   | LYS | A | 572 | 13.123 | 54.998 | 84.620 | 1.00 | 16.74 |
| ATOM | 4575 | CB  | LYS | A | 572 | 12.533 | 52.850 | 82.147 | 1.00 | 15.58 |
| ATOM | 4576 | CG  | LYS | A | 572 | 11.179 | 52.157 | 82.243 | 1.00 | 32.41 |
| ATOM | 4577 | CD  | LYS | A | 572 | 11.197 | 50.722 | 81.697 | 1.00 | 46.79 |
| ATOM | 4578 | CE  | LYS | A | 572 | 11.249 | 50.620 | 80.160 | 1.00 | 56.38 |
| ATOM | 4579 | NZ  | LYS | A | 572 | 11.823 | 49.373 | 79.593 | 1.00 | 42.31 |
| ATOM | 4580 | N   | ASP | A | 573 | 14.735 | 54.914 | 83.089 | 1.00 | 14.00 |
| ATOM | 4581 | CA  | ASP | A | 573 | 15.671 | 55.286 | 84.148 | 1.00 | 15.33 |
| ATOM | 4582 | C   | ASP | A | 573 | 15.394 | 56.675 | 84.662 | 1.00 | 15.63 |
| ATOM | 4583 | O   | ASP | A | 573 | 15.531 | 56.959 | 85.850 | 1.00 | 15.64 |
| ATOM | 4584 | CB  | ASP | A | 573 | 17.137 | 55.288 | 83.627 | 1.00 | 14.94 |
| ATOM | 4585 | CG  | ASP | A | 573 | 17.688 | 53.889 | 83.452 | 1.00 | 22.26 |
| ATOM | 4586 | OD1 | ASP | A | 573 | 17.054 | 52.891 | 83.773 | 1.00 | 18.66 |
| ATOM | 4587 | OD2 | ASP | A | 573 | 18.923 | 53.848 | 82.983 | 1.00 | 18.27 |
| ATOM | 4588 | N   | LEU | A | 574 | 15.090 | 57.554 | 83.708 | 1.00 | 12.68 |
| ATOM | 4589 | CA  | LEU | A | 574 | 14.851 | 58.926 | 84.092 | 1.00 | 11.33 |
| ATOM | 4590 | C   | LEU | A | 574 | 13.611 | 59.053 | 84.970 | 1.00 | 22.78 |
| ATOM | 4591 | O   | LEU | A | 574 | 13.513 | 59.923 | 85.837 | 1.00 | 18.71 |
| ATOM | 4592 | CB  | LEU | A | 574 | 14.682 | 59.802 | 82.863 | 1.00 | 10.39 |
| ATOM | 4593 | CG  | LEU | A | 574 | 15.953 | 60.021 | 82.061 | 1.00 | 16.41 |
| ATOM | 4594 | CD1 | LEU | A | 574 | 15.501 | 60.352 | 80.630 | 1.00 | 16.48 |
| ATOM | 4595 | CD2 | LEU | A | 574 | 16.785 | 61.200 | 82.608 | 1.00 | 12.08 |
| ATOM | 4596 | N   | ALA | A | 575 | 12.638 | 58.173 | 84.726 | 1.00 | 17.79 |
| ATOM | 4597 | CA  | ALA | A | 575 | 11.437 | 58.235 | 85.500 | 1.00 | 15.87 |
| ATOM | 4598 | C   | ALA | A | 575 | 11.720 | 57.682 | 86.856 | 1.00 | 17.98 |
| ATOM | 4599 | O   | ALA | A | 575 | 11.050 | 58.033 | 87.801 | 1.00 | 17.45 |
| ATOM | 4600 | CB  | ALA | A | 575 | 10.325 | 57.449 | 84.820 | 1.00 | 17.20 |
| ATOM | 4601 | N   | ALA | A | 576 | 12.703 | 56.801 | 86.972 | 1.00 | 14.91 |
| ATOM | 4602 | CA  | ALA | A | 576 | 13.024 | 56.222 | 88.272 | 1.00 | 12.59 |
| ATOM | 4603 | C   | ALA | A | 576 | 13.930 | 57.135 | 89.097 | 1.00 | 19.97 |
| ATOM | 4604 | O   | ALA | A | 576 | 14.140 | 56.920 | 90.281 | 1.00 | 22.87 |
| ATOM | 4605 | CB  | ALA | A | 576 | 13.732 | 54.881 | 88.146 | 1.00 | 16.01 |
| ATOM | 4606 | N   | PHE | A | 577 | 14.474 | 58.152 | 88.469 | 1.00 | 15.13 |
| ATOM | 4607 | CA  | PHE | A | 577 | 15.337 | 59.105 | 89.161 | 1.00 | 15.19 |
| ATOM | 4608 | C   | PHE | A | 577 | 14.412 | 60.219 | 89.660 | 1.00 | 19.07 |
| ATOM | 4609 | O   | PHE | A | 577 | 13.790 | 60.932 | 88.868 | 1.00 | 16.74 |
| ATOM | 4610 | CB  | PHE | A | 577 | 16.447 | 59.652 | 88.210 | 1.00 | 14.02 |
| ATOM | 4611 | CG  | PHE | A | 577 | 17.494 | 60.595 | 88.820 | 1.00 | 15.39 |
| ATOM | 4612 | CD1 | PHE | A | 577 | 17.678 | 60.707 | 90.202 | 1.00 | 17.32 |
| ATOM | 4613 | CD2 | PHE | A | 577 | 18.295 | 61.380 | 87.983 | 1.00 | 15.42 |
| ATOM | 4614 | CE1 | PHE | A | 577 | 18.646 | 61.570 | 90.727 | 1.00 | 18.05 |
| ATOM | 4615 | CE2 | PHE | A | 577 | 19.272 | 62.236 | 88.483 | 1.00 | 18.23 |
| ATOM | 4616 | CZ  | PHE | A | 577 | 19.442 | 62.330 | 89.866 | 1.00 | 18.02 |
| ATOM | 4617 | N   | ASP | A | 578 | 14.285 | 60.335 | 90.983 | 1.00 | 19.21 |
| ATOM | 4618 | CA  | ASP | A | 578 | 13.394 | 61.327 | 91.584 | 1.00 | 19.27 |
| ATOM | 4619 | C   | ASP | A | 578 | 13.568 | 62.692 | 90.981 | 1.00 | 18.95 |
| ATOM | 4620 | O   | ASP | A | 578 | 12.577 | 63.347 | 90.660 | 1.00 | 18.48 |
| ATOM | 4621 | CB  | ASP | A | 578 | 13.457 | 61.342 | 93.130 | 1.00 | 28.60 |
| ATOM | 4622 | CG  | ASP | A | 578 | 14.714 | 61.992 | 93.690 | 1.00 | 55.79 |
| ATOM | 4623 | OD1 | ASP | A | 578 | 15.779 | 62.135 | 93.064 | 1.00 | 45.74 |
| ATOM | 4624 | OD2 | ASP | A | 578 | 14.512 | 62.401 | 94.929 | 1.00 | 67.85 |
| ATOM | 4625 | N   | LYS | A | 579 | 14.839 | 63.083 | 90.791 | 1.00 | 17.12 |
| ATOM | 4626 | CA  | LYS | A | 579 | 15.185 | 64.352 | 90.194 | 1.00 | 13.88 |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 4627 | C   | LYS | A | 579 | 14.693 | 64.569 | 88.758 | 1.00 | 21.03 |
| ATOM | 4628 | O   | LYS | A | 579 | 14.338 | 65.689 | 88.386 | 1.00 | 20.91 |
| ATOM | 4629 | CB  | LYS | A | 579 | 16.669 | 64.621 | 90.293 | 1.00 | 13.46 |
| ATOM | 4630 | CG  | LYS | A | 579 | 17.159 | 64.570 | 91.724 | 1.00 | 33.01 |
| ATOM | 4631 | CD  | LYS | A | 579 | 16.890 | 65.878 | 92.442 | 1.00 | 55.78 |
| ATOM | 4632 | CE  | LYS | A | 579 | 16.292 | 65.662 | 93.816 | 1.00 | 58.11 |
| ATOM | 4633 | NZ  | LYS | A | 579 | 17.121 | 66.260 | 94.867 | 1.00 | 54.50 |
| ATOM | 4634 | N   | SER | A | 580 | 14.646 | 63.553 | 87.897 | 1.00 | 14.45 |
| ATOM | 4635 | CA  | SER | A | 580 | 14.187 | 63.844 | 86.540 | 1.00 | 13.57 |
| ATOM | 4636 | C   | SER | A | 580 | 12.798 | 63.298 | 86.228 | 1.00 | 20.81 |
| ATOM | 4637 | O   | SER | A | 580 | 12.313 | 63.384 | 85.103 | 1.00 | 19.66 |
| ATOM | 4638 | CB  | SER | A | 580 | 15.113 | 63.091 | 85.601 | 1.00 | 12.97 |
| ATOM | 4639 | OG  | SER | A | 580 | 15.350 | 61.809 | 86.186 | 1.00 | 17.95 |
| ATOM | 4640 | N   | HIS | A | 581 | 12.184 | 62.664 | 87.196 | 1.00 | 16.52 |
| ATOM | 4641 | CA  | HIS | A | 581 | 10.897 | 62.042 | 86.971 | 1.00 | 16.52 |
| ATOM | 4642 | C   | HIS | A | 581 | 9.816  | 62.866 | 86.281 | 1.00 | 21.39 |
| ATOM | 4643 | O   | HIS | A | 581 | 9.250  | 62.522 | 85.234 | 1.00 | 18.75 |
| ATOM | 4644 | CB  | HIS | A | 581 | 10.389 | 61.487 | 88.289 | 1.00 | 15.62 |
| ATOM | 4645 | CG  | HIS | A | 581 | 9.034  | 60.927 | 88.100 | 1.00 | 22.66 |
| ATOM | 4646 | ND1 | HIS | A | 581 | 7.914  | 61.748 | 88.110 | 1.00 | 27.83 |
| ATOM | 4647 | CD2 | HIS | A | 581 | 8.623  | 59.644 | 87.899 | 1.00 | 27.04 |
| ATOM | 4648 | CE1 | HIS | A | 581 | 6.843  | 60.975 | 87.926 | 1.00 | 27.26 |
| ATOM | 4649 | NE2 | HIS | A | 581 | 7.242  | 59.715 | 87.789 | 1.00 | 28.84 |
| ATOM | 4650 | N   | ASP | A | 582 | 9.515  | 63.986 | 86.884 | 1.00 | 17.59 |
| ATOM | 4651 | CA  | ASP | A | 582 | 8.491  | 64.831 | 86.322 | 1.00 | 20.99 |
| ATOM | 4652 | C   | ASP | A | 582 | 8.831  | 65.284 | 84.927 | 1.00 | 24.43 |
| ATOM | 4653 | O   | ASP | A | 582 | 8.013  | 65.343 | 84.030 | 1.00 | 21.69 |
| ATOM | 4654 | CB  | ASP | A | 582 | 8.331  | 66.085 | 87.197 | 1.00 | 25.08 |
| ATOM | 4655 | CG  | ASP | A | 582 | 7.626  | 65.730 | 88.466 | 1.00 | 30.98 |
| ATOM | 4656 | OD1 | ASP | A | 582 | 7.129  | 64.638 | 88.645 | 1.00 | 36.19 |
| ATOM | 4657 | OD2 | ASP | A | 582 | 7.659  | 66.680 | 89.359 | 1.00 | 38.67 |
| ATOM | 4658 | N   | GLN | A | 583 | 10.075 | 65.649 | 84.762 | 1.00 | 20.38 |
| ATOM | 4659 | CA  | GLN | A | 583 | 10.451 | 66.076 | 83.465 | 1.00 | 19.54 |
| ATOM | 4660 | C   | GLN | A | 583 | 10.423 | 64.938 | 82.431 | 1.00 | 23.45 |
| ATOM | 4661 | O   | GLN | A | 583 | 10.182 | 65.148 | 81.229 | 1.00 | 23.51 |
| ATOM | 4662 | CB  | GLN | A | 583 | 11.857 | 66.642 | 83.573 | 1.00 | 19.50 |
| ATOM | 4663 | CG  | GLN | A | 583 | 12.188 | 67.300 | 82.240 | 1.00 | 21.61 |
| ATOM | 4664 | CD  | GLN | A | 583 | 13.503 | 68.019 | 82.370 | 1.00 | 44.67 |
| ATOM | 4665 | OE1 | GLN | A | 583 | 14.236 | 67.818 | 83.357 | 1.00 | 39.11 |
| ATOM | 4666 | NE2 | GLN | A | 583 | 13.778 | 68.840 | 81.373 | 1.00 | 40.61 |
| ATOM | 4667 | N   | ALA | A | 584 | 10.706 | 63.718 | 82.866 | 1.00 | 18.70 |
| ATOM | 4668 | CA  | ALA | A | 584 | 10.700 | 62.595 | 81.927 | 1.00 | 15.00 |
| ATOM | 4669 | C   | ALA | A | 584 | 9.307  | 62.411 | 81.3   |      |       |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 4688 | NH1 | ARG | A | 586 | 9.767  | 69.873 | 82.357 | 1.00 | 50.55 |
| ATOM | 4689 | NH2 | ARG | A | 586 | 8.842  | 69.129 | 84.383 | 1.00 | 31.22 |
| ATOM | 4690 | N   | THR | A | 587 | 8.231  | 65.247 | 79.095 | 1.00 | 19.40 |
| ATOM | 4691 | CA  | THR | A | 587 | 8.856  | 65.157 | 77.781 | 1.00 | 18.84 |
| ATOM | 4692 | C   | THR | A | 587 | 8.150  | 64.170 | 76.882 | 1.00 | 20.71 |
| ATOM | 4693 | O   | THR | A | 587 | 7.885  | 64.391 | 75.702 | 1.00 | 23.03 |
| ATOM | 4694 | CB  | THR | A | 587 | 10.313 | 64.746 | 77.975 | 1.00 | 23.70 |
| ATOM | 4695 | OG1 | THR | A | 587 | 10.887 | 65.693 | 78.846 | 1.00 | 21.83 |
| ATOM | 4696 | CG2 | THR | A | 587 | 11.048 | 64.672 | 76.654 | 1.00 | 21.38 |
| ATOM | 4697 | N   | TYR | A | 588 | 7.822  | 63.043 | 77.464 | 1.00 | 21.74 |
| ATOM | 4698 | CA  | TYR | A | 588 | 7.137  | 62.033 | 76.693 | 1.00 | 19.43 |
| ATOM | 4699 | C   | TYR | A | 588 | 5.808  | 62.573 | 76.151 | 1.00 | 24.31 |
| ATOM | 4700 | O   | TYR | A | 588 | 5.450  | 62.483 | 74.963 | 1.00 | 26.68 |
| ATOM | 4701 | CB  | TYR | A | 588 | 6.846  | 60.854 | 77.638 | 1.00 | 18.46 |
| ATOM | 4702 | CG  | TYR | A | 588 | 5.842  | 59.904 | 77.014 | 1.00 | 21.76 |
| ATOM | 4703 | CD1 | TYR | A | 588 | 6.169  | 59.136 | 75.891 | 1.00 | 22.44 |
| ATOM | 4704 | CD2 | TYR | A | 588 | 4.549  | 59.808 | 77.540 | 1.00 | 22.19 |
| ATOM | 4705 | CE1 | TYR | A | 588 | 5.217  | 58.274 | 75.335 | 1.00 | 26.93 |
| ATOM | 4706 | CE2 | TYR | A | 588 | 3.584  | 58.961 | 76.999 | 1.00 | 19.19 |
| ATOM | 4707 | CZ  | TYR | A | 588 | 3.936  | 58.191 | 75.890 | 1.00 | 25.45 |
| ATOM | 4708 | OH  | TYR | A | 588 | 3.008  | 57.335 | 75.359 | 1.00 | 24.42 |
| ATOM | 4709 | N   | GLN | A | 589 | 5.039  | 63.110 | 77.088 | 1.00 | 23.42 |
| ATOM | 4710 | CA  | GLN | A | 589 | 3.727  | 63.642 | 76.762 | 1.00 | 22.93 |
| ATOM | 4711 | C   | GLN | A | 589 | 3.806  | 64.594 | 75.596 | 1.00 | 20.18 |
| ATOM | 4712 | O   | GLN | A | 589 | 2.957  | 64.626 | 74.707 | 1.00 | 23.55 |
| ATOM | 4713 | CB  | GLN | A | 589 | 3.139  | 64.384 | 77.981 | 1.00 | 25.07 |
| ATOM | 4714 | CG  | GLN | A | 589 | 2.683  | 63.449 | 79.119 | 1.00 | 21.54 |
| ATOM | 4715 | CD  | GLN | A | 589 | 1.470  | 62.587 | 78.765 | 1.00 | 41.81 |
| ATOM | 4716 | OE1 | GLN | A | 589 | 1.197  | 62.264 | 77.606 | 1.00 | 37.70 |
| ATOM | 4717 | NE2 | GLN | A | 589 | 0.721  | 62.186 | 79.779 | 1.00 | 58.94 |
| ATOM | 4718 | N   | GLU | A | 590 | 4.844  | 65.400 | 75.649 | 1.00 | 17.93 |
| ATOM | 4719 | CA  | GLU | A | 590 | 5.097  | 66.416 | 74.644 | 1.00 | 19.01 |
| ATOM | 4720 | C   | GLU | A | 590 | 5.566  | 65.826 | 73.363 | 1.00 | 26.93 |
| ATOM | 4721 | O   | GLU | A | 590 | 5.393  | 66.453 | 72.312 | 1.00 | 23.86 |
| ATOM | 4722 | CB  | GLU | A | 590 | 6.176  | 67.452 | 75.021 | 1.00 | 20.73 |
| ATOM | 4723 | CG  | GLU | A | 590 | 5.706  | 68.358 | 76.180 | 1.00 | 36.88 |
| ATOM | 4724 | CD  | GLU | A | 590 | 6.810  | 69.187 | 76.769 | 1.00 | 62.73 |
| ATOM | 4725 | OE1 | GLU | A | 590 | 7.988  | 69.112 | 76.403 | 1.00 | 55.19 |
| ATOM | 4726 | OE2 | GLU | A | 590 | 6.341  | 69.975 | 77.718 | 1.00 | 40.10 |
| ATOM | 4727 | N   | HIS | A | 591 | 6.203  | 64.666 | 73.476 | 1.00 | 23.79 |
| ATOM | 4728 | CA  | HIS | A | 591 | 6.700  | 64.086 | 72.250 | 1.00 | 23.24 |
| ATOM | 4729 | C   | HIS | A | 591 | 5.818  | 63.013 | 71.689 | 1.00 | 20.50 |
| ATOM | 4730 | O   | HIS | A | 591 | 5.965  | 62.619 | 70.541 |      |       |



|      |      |     |     |   |     |       |        |        |      |       |
|------|------|-----|-----|---|-----|-------|--------|--------|------|-------|
| ATOM | 4749 | O   | ALA | A | 593 | 2.741 | 62.121 | 66.732 | 1.00 | 28.39 |
| ATOM | 4750 | CB  | ALA | A | 593 | 1.558 | 64.018 | 68.998 | 1.00 | 24.94 |
| ATOM | 4751 | N   | SER | A | 594 | 4.420 | 62.891 | 67.988 | 1.00 | 21.56 |
| ATOM | 4752 | CA  | SER | A | 594 | 5.404 | 62.867 | 66.930 | 1.00 | 22.18 |
| ATOM | 4753 | C   | SER | A | 594 | 6.238 | 61.590 | 66.949 | 1.00 | 22.38 |
| ATOM | 4754 | O   | SER | A | 594 | 7.160 | 61.444 | 66.137 | 1.00 | 20.87 |
| ATOM | 4755 | CB  | SER | A | 594 | 6.352 | 64.049 | 67.098 | 1.00 | 29.27 |
| ATOM | 4756 | OG  | SER | A | 594 | 7.286 | 63.814 | 68.156 | 1.00 | 45.26 |
| ATOM | 4757 | N   | MET | A | 595 | 5.922 | 60.678 | 67.858 | 1.00 | 17.72 |
| ATOM | 4758 | CA  | MET | A | 595 | 6.732 | 59.453 | 67.945 | 1.00 | 17.90 |
| ATOM | 4759 | C   | MET | A | 595 | 6.240 | 58.295 | 67.114 | 1.00 | 21.9  |
| ATOM | 4760 | O   | MET | A | 595 | 5.105 | 58.257 | 66.683 | 1.00 | 26.36 |
| ATOM | 4761 | CB  | MET | A | 595 | 6.717 | 58.931 | 69.396 | 1.00 | 17.35 |
| ATOM | 4762 | CG  | MET | A | 595 | 7.616 | 59.720 | 70.321 | 1.00 | 18.64 |
| ATOM | 4763 | SD  | MET | A | 595 | 7.451 | 59.068 | 71.999 | 1.00 | 25.54 |
| ATOM | 4764 | CE  | MET | A | 595 | 7.775 | 60.523 | 72.990 | 1.00 | 32.21 |
| ATOM | 4765 | N   | HIS | A | 596 | 7.066 | 57.284 | 66.954 | 1.00 | 15.02 |
| ATOM | 4766 | CA  | HIS | A | 596 | 6.593 | 56.105 | 66.258 | 1.00 | 16.62 |
| ATOM | 4767 | C   | HIS | A | 596 | 5.458 | 55.524 | 67.111 | 1.00 | 19.77 |
| ATOM | 4768 | O   | HIS | A | 596 | 5.474 | 55.605 | 68.324 | 1.00 | 19.53 |
| ATOM | 4769 | CB  | HIS | A | 596 | 7.756 | 55.103 | 66.052 | 1.00 | 17.44 |
| ATOM | 4770 | CG  | HIS | A | 596 | 7.280 | 53.844 | 65.414 | 1.00 | 20.36 |
| ATOM | 4771 | ND1 | HIS | A | 596 | 7.474 | 53.623 | 64.059 | 1.00 | 22.76 |
| ATOM | 4772 | CD2 | HIS | A | 596 | 6.582 | 52.790 | 65.937 | 1.00 | 19.37 |
| ATOM | 4773 | CE1 | HIS | A | 596 | 6.928 | 52.443 | 63.770 | 1.00 | 21.23 |
| ATOM | 4774 | NE2 | HIS | A | 596 | 6.375 | 51.935 | 64.879 | 1.00 | 22.61 |
| ATOM | 4775 | N   | PRO | A | 597 | 4.425 | 54.948 | 66.507 | 1.00 | 19.72 |
| ATOM | 4776 | CA  | PRO | A | 597 | 3.284 | 54.409 | 67.233 | 1.00 | 17.32 |
| ATOM | 4777 | C   | PRO | A | 597 | 3.515 | 53.268 | 68.221 | 1.00 | 22.24 |
| ATOM | 4778 | O   | PRO | A | 597 | 2.887 | 53.165 | 69.277 | 1.00 | 20.86 |
| ATOM | 4779 | CB  | PRO | A | 597 | 2.228 | 54.031 | 66.181 | 1.00 | 15.13 |
| ATOM | 4780 | CG  | PRO | A | 597 | 2.989 | 53.918 | 64.893 | 1.00 | 20.16 |
| ATOM | 4781 | CD  | PRO | A | 597 | 4.195 | 54.843 | 65.045 | 1.00 | 19.53 |
| ATOM | 4782 | N   | VAL | A | 598 | 4.381 | 52.340 | 67.895 | 1.00 | 17.95 |
| ATOM | 4783 | CA  | VAL | A | 598 | 4.575 | 51.277 | 68.868 | 1.00 | 17.06 |
| ATOM | 4784 | C   | VAL | A | 598 | 5.463 | 51.830 | 69.993 | 1.00 | 16.39 |
| ATOM | 4785 | O   | VAL | A | 598 | 5.188 | 51.629 | 71.176 | 1.00 | 18.72 |
| ATOM | 4786 | CB  | VAL | A | 598 | 5.175 | 50.039 | 68.180 | 1.00 | 20.87 |
| ATOM | 4787 | CG1 | VAL | A | 598 | 5.739 | 48.974 | 69.142 | 1.00 | 15.98 |
| ATOM | 4788 | CG2 | VAL | A | 598 | 4.169 | 49.498 | 67.132 | 1.00 | 17.75 |
| ATOM | 4789 | N   | THR | A | 599 | 6.521 | 52.548 | 69.605 | 1.00 | 17.91 |
| ATOM | 4790 | CA  | THR | A | 599 | 7.370 | 53.125 | 70.636 | 1.00 | 20.42 |
| ATOM | 4791 | C   | THR | A | 599 | 6.544 | 53.965 | 71.615 | 1.00 | 25.40 |
| ATOM | 4792 | O   |     |   |     |       |        |        |      |       |



|      |      |     |     |   |     |       |        |        |      |       |
|------|------|-----|-----|---|-----|-------|--------|--------|------|-------|
| ATOM | 4810 | CA  | LEU | A | 602 | 5.389 | 51.117 | 74.924 | 1.00 | 16.19 |
| ATOM | 4811 | C   | LEU | A | 602 | 5.940 | 52.055 | 76.027 | 1.00 | 18.15 |
| ATOM | 4812 | O   | LEU | A | 602 | 5.962 | 51.722 | 77.214 | 1.00 | 18.36 |
| ATOM | 4813 | CB  | LEU | A | 602 | 6.507 | 50.267 | 74.269 | 1.00 | 14.21 |
| ATOM | 4814 | CG  | LEU | A | 602 | 5.987 | 49.058 | 73.508 | 1.00 | 18.02 |
| ATOM | 4815 | CD1 | LEU | A | 602 | 7.100 | 48.467 | 72.642 | 1.00 | 17.78 |
| ATOM | 4816 | CD2 | LEU | A | 602 | 5.502 | 48.030 | 74.515 | 1.00 | 21.84 |
| ATOM | 4817 | N   | VAL | A | 603 | 6.426 | 53.224 | 75.617 | 1.00 | 15.71 |
| ATOM | 4818 | CA  | VAL | A | 603 | 6.962 | 54.208 | 76.549 | 1.00 | 15.67 |
| ATOM | 4819 | C   | VAL | A | 603 | 5.877 | 54.648 | 77.537 | 1.00 | 17.35 |
| ATOM | 4820 | O   | VAL | A | 603 | 6.093 | 54.733 | 78.741 | 1.00 | 18.72 |
| ATOM | 4821 | CB  | VAL | A | 603 | 7.665 | 55.345 | 75.807 | 1.00 | 19.16 |
| ATOM | 4822 | CG1 | VAL | A | 603 | 8.035 | 56.477 | 76.764 | 1.00 | 15.61 |
| ATOM | 4823 | CG2 | VAL | A | 603 | 8.943 | 54.837 | 75.115 | 1.00 | 17.56 |
| ATOM | 4824 | N   | GLY | A | 604 | 4.661 | 54.851 | 77.027 | 1.00 | 14.92 |
| ATOM | 4825 | CA  | GLY | A | 604 | 3.535 | 55.262 | 77.879 | 1.00 | 14.02 |
| ATOM | 4826 | C   | GLY | A | 604 | 3.239 | 54.206 | 78.898 | 1.00 | 17.85 |
| ATOM | 4827 | O   | GLY | A | 604 | 2.984 | 54.443 | 80.075 | 1.00 | 21.21 |
| ATOM | 4828 | N   | LYS | A | 605 | 3.306 | 52.987 | 78.426 | 1.00 | 16.57 |
| ATOM | 4829 | CA  | LYS | A | 605 | 3.127 | 51.873 | 79.330 | 1.00 | 18.08 |
| ATOM | 4830 | C   | LYS | A | 605 | 4.251 | 51.892 | 80.348 | 1.00 | 22.76 |
| ATOM | 4831 | O   | LYS | A | 605 | 4.034 | 51.859 | 81.558 | 1.00 | 26.27 |
| ATOM | 4832 | CB  | LYS | A | 605 | 3.190 | 50.541 | 78.607 | 1.00 | 22.73 |
| ATOM | 4833 | CG  | LYS | A | 605 | 1.870 | 49.811 | 78.714 | 1.00 | 40.15 |
| ATOM | 4834 | CD  | LYS | A | 605 | 1.919 | 48.377 | 78.211 | 1.00 | 57.40 |
| ATOM | 4835 | CE  | LYS | A | 605 | 1.068 | 47.461 | 79.074 | 1.00 | 75.31 |
| ATOM | 4836 | NZ  | LYS | A | 605 | 1.808 | 46.387 | 79.758 | 1.00 | 74.64 |
| ATOM | 4837 | N   | ASP | A | 606 | 5.470 | 51.943 | 79.836 | 1.00 | 17.17 |
| ATOM | 4838 | CA  | ASP | A | 606 | 6.607 | 51.972 | 80.718 | 1.00 | 16.61 |
| ATOM | 4839 | C   | ASP | A | 606 | 6.442 | 53.059 | 81.738 | 1.00 | 19.46 |
| ATOM | 4840 | O   | ASP | A | 606 | 6.790 | 52.848 | 82.884 | 1.00 | 19.57 |
| ATOM | 4841 | CB  | ASP | A | 606 | 7.945 | 52.255 | 79.990 | 1.00 | 16.98 |
| ATOM | 4842 | CG  | ASP | A | 606 | 8.365 | 51.063 | 79.187 | 1.00 | 21.21 |
| ATOM | 4843 | OD1 | ASP | A | 606 | 7.944 | 49.933 | 79.376 | 1.00 | 20.21 |
| ATOM | 4844 | OD2 | ASP | A | 606 | 9.189 | 51.355 | 78.249 | 1.00 | 18.07 |
| ATOM | 4845 | N   | LEU | A | 607 | 5.974 | 54.207 | 81.306 | 1.00 | 16.61 |
| ATOM | 4846 | CA  | LEU | A | 607 | 5.863 | 55.352 | 82.211 | 1.00 | 20.64 |
| ATOM | 4847 | C   | LEU | A | 607 | 4.586 | 55.384 | 83.026 | 1.00 | 27.05 |
| ATOM | 4848 | O   | LEU | A | 607 | 4.361 | 56.274 | 83.862 | 1.00 | 23.83 |
| ATOM | 4849 | CB  | LEU | A | 607 | 5.991 | 56.641 | 81.388 | 1.00 | 23.11 |
| ATOM | 4850 | CG  | LEU | A | 607 | 7.377 | 57.301 | 81.464 | 1.00 | 28.84 |
| ATOM | 4851 | CD1 | LEU | A | 607 | 8.508 | 56.323 | 81.711 | 1.00 | 29.33 |
| ATOM | 4852 | CD2 | LEU | A | 607 | 7.650 | 58.116 | 80.214 | 1.00 |       |



|      |      |      |     |   |     |         |        |        |            |
|------|------|------|-----|---|-----|---------|--------|--------|------------|
| ATOM | 4871 | C    | ASP | A | 610 | -3.541  | 56.207 | 81.365 | 1.00100.00 |
| ATOM | 4872 | O    | ASP | A | 610 | -3.950  | 56.568 | 82.470 | 1.00 78.31 |
| ATOM | 4873 | CB   | ASP | A | 610 | -2.550  | 56.631 | 79.044 | 1.00100.00 |
| ATOM | 4874 | CG   | ASP | A | 610 | -1.930  | 57.631 | 78.091 | 1.00100.00 |
| ATOM | 4875 | OD1  | ASP | A | 610 | -2.251  | 58.807 | 78.062 | 1.00 99.48 |
| ATOM | 4876 | OD2  | ASP | A | 610 | -1.019  | 57.111 | 77.288 | 1.00100.00 |
| TER  | 4877 |      | ASP | A | 610 |         |        |        |            |
| ATOM | 4878 | ZN2+ | ZN  | Z | 1   | 16.972  | 39.340 | 64.102 | 1.00 16.33 |
| ATOM | 4879 | YB3+ | YB  | Y | 1   | 42.669  | 51.366 | 99.201 | 1.00 18.06 |
| ATOM | 4880 | YB3+ | YB  | Y | 2   | -13.732 | 57.497 | 52.155 | 0.50 46.53 |
| ATOM | 4881 | YB3+ | YB  | Y | 3   | -10.443 | 58.443 | 52.469 | 0.50 30.25 |
| ATOM | 4882 | N2   | BES | B | 1   | 13.712  | 41.186 | 63.145 | 1.00 25.72 |
| ATOM | 4883 | C1   | BES | B | 1   | 14.450  | 41.733 | 64.255 | 1.00 24.13 |
| ATOM | 4884 | C6   | BES | B | 1   | 13.749  | 42.939 | 64.880 | 1.00 23.84 |
| ATOM | 4885 | C7   | BES | B | 1   | 12.300  | 42.727 | 65.283 | 1.00 19.51 |
| ATOM | 4886 | C8   | BES | B | 1   | 11.297  | 43.571 | 64.799 | 1.00 18.42 |
| ATOM | 4887 | C12  | BES | B | 1   | 11.934  | 41.717 | 66.170 | 1.00 19.27 |
| ATOM | 4888 | C9   | BES | B | 1   | 9.990   | 43.454 | 65.227 | 1.00 16.90 |
| ATOM | 4889 | C11  | BES | B | 1   | 10.614  | 41.580 | 66.600 | 1.00 19.17 |
| ATOM | 4890 | C10  | BES | B | 1   | 9.639   | 42.451 | 66.135 | 1.00 18.42 |
| ATOM | 4891 | C2   | BES | B | 1   | 15.881  | 42.065 | 63.795 | 1.00 21.80 |
| ATOM | 4892 | O2   | BES | B | 1   | 16.369  | 41.004 | 62.999 | 1.00 18.60 |
| ATOM | 4893 | C3   | BES | B | 1   | 16.741  | 42.156 | 65.063 | 1.00 23.33 |
| ATOM | 4894 | O3   | BES | B | 1   | 16.932  | 41.185 | 65.803 | 1.00 25.68 |
| ATOM | 4895 | N1   | BES | B | 1   | 17.280  | 43.376 | 65.250 | 1.00 21.90 |
| ATOM | 4896 | C4   | BES | B | 1   | 18.157  | 43.613 | 66.390 | 1.00 24.18 |
| ATOM | 4897 | C13  | BES | B | 1   | 19.568  | 43.595 | 65.855 | 1.00 22.49 |
| ATOM | 4898 | C14  | BES | B | 1   | 20.669  | 42.812 | 66.576 | 1.00 24.23 |
| ATOM | 4899 | C15  | BES | B | 1   | 20.210  | 41.770 | 67.577 | 1.00 23.32 |
| ATOM | 4900 | C16  | BES | B | 1   | 21.692  | 42.287 | 65.590 | 1.00 22.52 |
| ATOM | 4901 | C5   | BES | B | 1   | 17.840  | 45.000 | 67.053 | 1.00 25.70 |
| ATOM | 4902 | O1   | BES | B | 1   | 17.160  | 45.848 | 66.348 | 1.00 22.63 |
| ATOM | 4903 | O4   | BES | B | 1   | 18.206  | 45.226 | 68.192 | 1.00 26.52 |
| ATOM | 4904 | CG   | IMD | I | 1   | 26.142  | 42.633 | 80.576 | 1.00 14.44 |
| ATOM | 4905 | ND1  | IMD | I | 1   | 25.962  | 42.811 | 79.218 | 1.00 15.15 |
| ATOM | 4906 | CD2  | IMD | I | 1   | 27.444  | 42.291 | 80.744 | 1.00 13.81 |
| ATOM | 4907 | CE1  | IMD | I | 1   | 27.096  | 42.555 | 78.588 | 1.00 9.17  |
| ATOM | 4908 | NE2  | IMD | I | 1   | 28.014  | 42.249 | 79.494 | 1.00 21.14 |
| ATOM | 4909 | CB   | ACE | C | 1   | 13.753  | 12.531 | 68.686 | 1.00 39.29 |
| ATOM | 4910 | CG   | ACE | C | 1   | 13.041  | 13.755 | 69.176 | 1.00 52.31 |
| ATOM | 4911 | OD1  | ACE | C | 1   | 13.310  | 14.951 | 68.885 | 1.00 21.34 |
| ATOM | 4912 | OD2  | ACE | C | 1   | 12.075  | 13.324 | 69.958 | 1.00 27.10 |
| ATOM | 4913 | O    | HOH | W | 1   | 23.792  | 34.258 | 75.188 | 1.00 13.41 |
| ATOM | 4914 | O    | HOH | W | 2   | 41.402  | 41.645 | 77.736 | 1.00 18.41 |
| ATOM | 4915 | O    | HOH | W | 3   | 21.452  | 48.008 | 79.289 | 1.00 14.29 |
| ATOM | 4916 | O    | HOH | W | 4   | 7.395   | 22.508 | 68.980 | 1.00 15.42 |
| ATOM | 4917 | O    | HOH | W | 5   | 8.875   | 45.610 | 71.521 | 1.00 15.01 |
| ATOM | 4918 | O    | HOH | W | 6   | 18.318  | 15.775 | 81.560 | 1.00 42.99 |
| ATOM | 4919 | O    | HOH | W | 7   | 30.607  | 45.406 | 73.230 | 1.00 16.49 |
| ATOM | 4920 | O    | HOH | W | 8   | 2.151   | 35.326 | 56.132 | 1.00 20.69 |
| ATOM | 4921 | O    | HOH | W | 9   | 26.371  | 45.237 | 72.729 | 1.00 32.21 |
| ATOM | 4922 | O    | HOH | W | 10  | 10.117  | 47.411 | 58.465 | 1.00 19.66 |
| ATOM | 4923 | O    | HOH | W | 11  | 24.576  | 45.901 | 81.764 | 1.00 15.98 |
| ATOM | 4924 | O    | HOH | W | 12  | 21.400  | 39.522 | 70.350 | 1.00 17.59 |
| ATOM | 4925 | O    | HOH | W | 13  | 32.755  | 39.688 | 76.763 | 1.00 14.73 |
| ATOM | 4926 | O    | HOH | W | 14  | 15.723  | 43.292 | 73.593 | 1.00 28.15 |
| ATOM | 4927 | O    | HOH | W | 15  | 33.012  | 53.990 | 68.029 | 1.00 20.61 |
| ATOM | 4928 | O    | HOH | W | 16  | 21.672  | 48.368 | 86.318 | 1.00 18.35 |
| ATOM | 4929 | O    | HOH | W | 17  | 11.843  | 66.293 | 86.775 | 1.00 20.28 |
| ATOM | 4930 | O    | HOH | W | 18  | -7.370  | 39.258 | 72.858 | 1.00100.00 |
| ATOM | 4931 | O    | HOH | W | 19  | 10.951  | 58.853 | 90.712 | 1.00 31.18 |



|      |      |   |     |   |    |        |        |          |      |       |
|------|------|---|-----|---|----|--------|--------|----------|------|-------|
| ATOM | 4932 | O | HOH | W | 20 | 7.991  | 67.991 | 69.688   | 1.00 | 51.29 |
| ATOM | 4933 | O | HOH | W | 21 | 27.534 | 25.933 | 83.686   | 1.00 | 30.42 |
| ATOM | 4934 | O | HOH | W | 22 | 14.754 | 47.886 | 81.192   | 1.00 | 91.59 |
| ATOM | 4935 | O | HOH | W | 23 | 35.638 | 66.681 | 74.616   | 1.00 | 18.43 |
| ATOM | 4936 | O | HOH | W | 24 | 14.917 | 46.651 | 71.292   | 1.00 | 29.09 |
| ATOM | 4937 | O | HOH | W | 25 | 24.339 | 72.545 | 82.858   | 1.00 | 27.38 |
| ATOM | 4938 | O | HOH | W | 26 | 3.954  | 59.653 | 64.218   | 1.00 | 29.75 |
| ATOM | 4939 | O | HOH | W | 27 | 0.174  | 30.326 | 72.099   | 1.00 | 20.53 |
| ATOM | 4940 | O | HOH | W | 28 | 17.250 | 55.520 | 87.251   | 1.00 | 15.14 |
| ATOM | 4941 | O | HOH | W | 29 | 2.640  | 38.007 | 61.525   | 1.00 | 15.01 |
| ATOM | 4942 | O | HOH | W | 30 | 10.861 | 36.115 | 89.266   | 1.00 | 26.76 |
| ATOM | 4943 | O | HOH | W | 31 | 30.988 | 44.243 | 70.800   | 1.00 | 37.98 |
| ATOM | 4944 | O | HOH | W | 32 | 9.095  | 44.675 | 75.314   | 1.00 | 24.97 |
| ATOM | 4945 | O | HOH | W | 33 | 29.917 | 47.569 | 70.312   | 1.00 | 33.43 |
| ATOM | 4946 | O | HOH | W | 34 | 23.537 | 45.186 | 73.070   | 1.00 | 21.89 |
| ATOM | 4947 | O | HOH | W | 35 | 13.919 | 30.086 | 87.520   | 1.00 | 27.60 |
| ATOM | 4948 | O | HOH | W | 36 | 24.004 | 28.230 | 84.950   | 1.00 | 54.91 |
| ATOM | 4949 | O | HOH | W | 37 | 44.740 | 56.907 | 93.797   | 1.00 | 39.70 |
| ATOM | 4950 | O | HOH | W | 38 | 36.453 | 36.919 | 75.700   | 1.00 | 12.06 |
| ATOM | 4951 | O | HOH | W | 39 | 27.587 | 65.302 | 75.920   | 1.00 | 21.02 |
| ATOM | 4952 | O | HOH | W | 40 | 23.077 | 39.811 | 87.155   | 1.00 | 38.48 |
| ATOM | 4953 | O | HOH | W | 41 | 3.661  | 37.055 | 59.039   | 1.00 | 17.86 |
| ATOM | 4954 | O | HOH | W | 42 | 21.794 | 20.673 | 79.219   | 1.00 | 20.60 |
| ATOM | 4955 | O | HOH | W | 43 | 6.324  | 36.055 | 87.167   | 1.00 | 30.35 |
| ATOM | 4956 | O | HOH | W | 44 | 24.649 | 34.194 | 44.975   | 1.00 | 52.51 |
| ATOM | 4957 | O | HOH | W | 45 | 20.611 | 44.717 | 78.685   | 1.00 | 27.41 |
| ATOM | 4958 | O | HOH | W | 46 | 19.969 | 50.884 | 89.461   | 1.00 | 29.62 |
| ATOM | 4959 | O | HOH | W | 47 | 30.940 | 66.808 | 78.811   | 1.00 | 15.76 |
| ATOM | 4960 | O | HOH | W | 48 | 26.539 | 55.260 | 66.886   | 1.00 | 19.97 |
| ATOM | 4961 | O | HOH | W | 49 | 7.314  | 45.436 | 77.867   | 1.00 | 35.07 |
| ATOM | 4962 | O | HOH | W | 50 | 10.579 | 54.800 | 67.603   | 1.00 | 15.62 |
| ATOM | 4963 | O | HOH | W | 51 | 28.138 | 31.371 | 66.611   | 1.00 | 15.08 |
| ATOM | 4964 | O | HOH | W | 52 | 26.292 | 33.348 | 75.129   | 1.00 | 15.49 |
| ATOM | 4965 | O | HOH | W | 53 | 15.204 | 48.508 | 69.331   | 1.00 | 16.03 |
| ATOM | 4966 | O | HOH | W | 54 | 9.451  | 57.282 | 68.158   | 1.00 | 20.39 |
| ATOM | 4967 | O | HOH | W | 55 | 34.923 | 67.738 | 77.001   | 1.00 | 15.06 |
| ATOM | 4968 | O | HOH | W | 56 | 10.193 | 53.763 | 78.443   | 1.00 | 19.23 |
| ATOM | 4969 | O | HOH | W | 57 | 35.246 | 32.562 | 64.227   | 1.00 | 27.89 |
| ATOM | 4970 | O | HOH | W | 58 | 7.230  | 48.517 | 65.509   | 1.00 | 17.57 |
| ATOM | 4971 | O | HOH | W | 59 | 15.707 | 29.269 | 62.146   | 1.00 | 16.76 |
| ATOM | 4972 | O | HOH | W | 60 | 22.703 | 46.209 | 83.610   | 1.00 | 14.72 |
| ATOM | 4973 | O | HOH | W | 61 | -5.573 | 31.742 | 67.048   | 1.00 | 67.53 |
| ATOM | 4974 | O | HOH | W | 62 | 23.958 | 46.448 | 79.118</ |      |       |



|      |      |   |     |   |     |        |        |        |      |       |
|------|------|---|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 4993 | O | HOH | W | 81  | 5.222  | 49.330 | 63.415 | 1.00 | 17.36 |
| ATOM | 4994 | O | HOH | W | 82  | 16.211 | 37.941 | 52.836 | 1.00 | 19.88 |
| ATOM | 4995 | O | HOH | W | 83  | 32.789 | 43.179 | 86.654 | 1.00 | 20.34 |
| ATOM | 4996 | O | HOH | W | 84  | 9.298  | 48.075 | 81.153 | 1.00 | 54.83 |
| ATOM | 4997 | O | HOH | W | 85  | 29.454 | 36.152 | 82.527 | 1.00 | 29.31 |
| ATOM | 4998 | O | HOH | W | 86  | 41.926 | 50.859 | 91.024 | 1.00 | 26.91 |
| ATOM | 4999 | O | HOH | W | 87  | 42.353 | 47.486 | 84.905 | 1.00 | 21.77 |
| ATOM | 5000 | O | HOH | W | 88  | 7.099  | 45.738 | 66.261 | 1.00 | 16.80 |
| ATOM | 5001 | O | HOH | W | 89  | -7.189 | 40.950 | 62.864 | 1.00 | 18.87 |
| ATOM | 5002 | O | HOH | W | 90  | -0.532 | 35.957 | 55.006 | 1.00 | 30.96 |
| ATOM | 5003 | O | HOH | W | 91  | 2.498  | 58.239 | 62.223 | 1.00 | 33.64 |
| ATOM | 5004 | O | HOH | W | 92  | 8.030  | 54.347 | 85.172 | 1.00 | 36.67 |
| ATOM | 5005 | O | HOH | W | 93  | -9.086 | 47.257 | 64.010 | 1.00 | 25.14 |
| ATOM | 5006 | O | HOH | W | 94  | 7.634  | 23.157 | 71.565 | 1.00 | 26.48 |
| ATOM | 5007 | O | HOH | W | 95  | 36.802 | 57.687 | 75.942 | 1.00 | 33.51 |
| ATOM | 5008 | O | HOH | W | 96  | 31.266 | 28.847 | 81.561 | 1.00 | 33.78 |
| ATOM | 5009 | O | HOH | W | 97  | 42.718 | 53.265 | 90.455 | 1.00 | 18.15 |
| ATOM | 5010 | O | HOH | W | 98  | 25.175 | 49.362 | 94.064 | 1.00 | 38.55 |
| ATOM | 5011 | O | HOH | W | 99  | -1.458 | 36.897 | 71.377 | 1.00 | 21.47 |
| ATOM | 5012 | O | HOH | W | 100 | 36.955 | 22.462 | 67.101 | 1.00 | 62.30 |
| ATOM | 5013 | O | HOH | W | 101 | 17.777 | 47.785 | 75.841 | 1.00 | 20.17 |
| ATOM | 5014 | O | HOH | W | 102 | 17.194 | 41.841 | 54.112 | 1.00 | 16.39 |
| ATOM | 5015 | O | HOH | W | 103 | -1.972 | 55.370 | 57.254 | 1.00 | 25.11 |
| ATOM | 5016 | O | HOH | W | 104 | 27.602 | 40.677 | 72.586 | 1.00 | 21.30 |
| ATOM | 5017 | O | HOH | W | 105 | 37.435 | 51.467 | 61.104 | 1.00 | 65.38 |
| ATOM | 5018 | O | HOH | W | 106 | 1.256  | 32.447 | 69.628 | 1.00 | 23.44 |
| ATOM | 5019 | O | HOH | W | 107 | 9.241  | 16.192 | 63.327 | 1.00 | 48.00 |
| ATOM | 5020 | O | HOH | W | 108 | 0.854  | 36.054 | 64.035 | 1.00 | 18.60 |
| ATOM | 5021 | O | HOH | W | 109 | 18.727 | 44.131 | 84.651 | 1.00 | 24.89 |
| ATOM | 5022 | O | HOH | W | 110 | 26.098 | 18.961 | 78.803 | 1.00 | 24.48 |
| ATOM | 5023 | O | HOH | W | 111 | 19.158 | 42.699 | 78.273 | 1.00 | 28.07 |
| ATOM | 5024 | O | HOH | W | 112 | 38.525 | 39.961 | 90.164 | 1.00 | 49.63 |
| ATOM | 5025 | O | HOH | W | 113 | 18.603 | 45.487 | 82.264 | 1.00 | 21.64 |
| ATOM | 5026 | O | HOH | W | 114 | -9.935 | 47.106 | 60.568 | 1.00 | 27.24 |
| ATOM | 5027 | O | HOH | W | 115 | 12.837 | 36.710 | 59.433 | 1.00 | 15.13 |
| ATOM | 5028 | O | HOH | W | 116 | 33.438 | 65.032 | 85.997 | 1.00 | 32.21 |
| ATOM | 5029 | O | HOH | W | 117 | 38.122 | 36.535 | 73.494 | 1.00 | 12.50 |
| ATOM | 5030 | O | HOH | W | 118 | 39.258 | 66.537 | 78.047 | 1.00 | 18.65 |
| ATOM | 5031 | O | HOH | W | 119 | 6.554  | 34.671 | 88.987 | 1.00 | 15.86 |
| ATOM | 5032 | O | HOH | W | 120 | 13.095 | 46.874 | 73.346 | 1.00 | 30.35 |
| ATOM | 5033 | O | HOH | W | 121 | 32.660 | 36.335 | 82.732 | 1.00 | 35.47 |
| ATOM | 5034 | O | HOH | W | 122 | 9.605  | 28.610 | 88.505 | 1.00 | 19.15 |
| ATOM | 5035 | O | HOH | W | 123 | 27.330 |        |        |      |       |



|      |      |   |     |       |         |        |        |      |       |
|------|------|---|-----|-------|---------|--------|--------|------|-------|
| ATOM | 5054 | O | HOH | W 142 | 25.840  | 58.036 | 65.771 | 1.00 | 54.37 |
| ATOM | 5055 | O | HOH | W 143 | 10.922  | 53.966 | 85.792 | 1.00 | 18.98 |
| ATOM | 5056 | O | HOH | W 144 | -12.182 | 45.374 | 45.449 | 1.00 | 33.96 |
| ATOM | 5057 | O | HOH | W 145 | 31.206  | 39.579 | 79.369 | 1.00 | 15.60 |
| ATOM | 5058 | O | HOH | W 146 | 15.440  | 42.222 | 77.590 | 1.00 | 25.43 |
| ATOM | 5059 | O | HOH | W 147 | 0.824   | 56.052 | 62.386 | 1.00 | 26.41 |
| ATOM | 5060 | O | HOH | W 148 | 44.978  | 53.578 | 86.262 | 1.00 | 22.60 |
| ATOM | 5061 | O | HOH | W 149 | 17.898  | 31.967 | 86.834 | 1.00 | 19.51 |
| ATOM | 5062 | O | HOH | W 150 | 15.892  | 63.944 | 61.374 | 1.00 | 54.27 |
| ATOM | 5063 | O | HOH | W 151 | 29.311  | 44.330 | 75.316 | 1.00 | 39.02 |
| ATOM | 5064 | O | HOH | W 152 | 11.678  | 62.566 | 52.561 | 1.00 | 27.61 |
| ATOM | 5065 | O | HOH | W 153 | 26.748  | 53.479 | 95.785 | 1.00 | 45.53 |
| ATOM | 5066 | O | HOH | W 154 | 35.164  | 39.157 | 88.454 | 1.00 | 33.28 |
| ATOM | 5067 | O | HOH | W 155 | 13.599  | 30.411 | 61.539 | 1.00 | 16.55 |
| ATOM | 5068 | O | HOH | W 156 | 2.955   | 41.496 | 60.167 | 1.00 | 26.41 |
| ATOM | 5069 | O | HOH | W 157 | 21.013  | 47.058 | 81.902 | 1.00 | 24.07 |
| ATOM | 5070 | O | HOH | W 158 | 7.082   | 15.804 | 68.963 | 1.00 | 13.64 |
| ATOM | 5071 | O | HOH | W 159 | 43.659  | 51.565 | 97.228 | 1.00 | 13.91 |
| ATOM | 5072 | O | HOH | W 160 | 25.728  | 46.521 | 67.857 | 1.00 | 15.18 |
| ATOM | 5073 | O | HOH | W 161 | 16.336  | 27.429 | 80.519 | 1.00 | 13.58 |
| ATOM | 5074 | O | HOH | W 162 | 13.506  | 27.963 | 78.488 | 1.00 | 11.63 |
| ATOM | 5075 | O | HOH | W 163 | -1.826  | 28.836 | 60.633 | 1.00 | 18.21 |
| ATOM | 5076 | O | HOH | W 164 | 2.041   | 28.523 | 68.718 | 1.00 | 19.80 |
| ATOM | 5077 | O | HOH | W 165 | 39.832  | 50.082 | 92.567 | 1.00 | 15.76 |
| ATOM | 5078 | O | HOH | W 166 | 20.417  | 35.797 | 44.686 | 1.00 | 23.98 |
| ATOM | 5079 | O | HOH | W 167 | 36.272  | 60.259 | 74.993 | 1.00 | 26.08 |
| ATOM | 5080 | O | HOH | W 168 | 5.426   | 61.205 | 63.338 | 1.00 | 23.06 |
| ATOM | 5081 | O | HOH | W 169 | 17.667  | 67.608 | 77.116 | 1.00 | 28.66 |
| ATOM | 5082 | O | HOH | W 170 | 5.631   | 18.160 | 69.508 | 1.00 | 19.48 |
| ATOM | 5083 | O | HOH | W 171 | 22.328  | 62.979 | 93.415 | 1.00 | 25.81 |
| ATOM | 5084 | O | HOH | W 172 | 40.390  | 48.175 | 94.855 | 1.00 | 47.37 |
| ATOM | 5085 | O | HOH | W 173 | 17.444  | 40.095 | 51.789 | 1.00 | 18.19 |
| ATOM | 5086 | O | HOH | W 174 | 29.587  | 24.011 | 76.681 | 1.00 | 24.09 |
| ATOM | 5087 | O | HOH | W 175 | 6.778   | 26.010 | 80.637 | 1.00 | 26.64 |
| ATOM | 5088 | O | HOH | W 176 | 43.821  | 42.250 | 81.895 | 1.00 | 24.88 |
| ATOM | 5089 | O | HOH | W 177 | 28.198  | 18.300 | 60.474 | 1.00 | 24.14 |
| ATOM | 5090 | O | HOH | W 178 | 22.788  | 46.771 | 90.209 | 1.00 | 24.26 |
| ATOM | 5091 | O | HOH | W 179 | 29.931  | 24.564 | 79.534 | 1.00 | 31.74 |
| ATOM | 5092 | O | HOH | W 180 | 10.739  | 18.587 | 70.209 | 1.00 | 34.82 |
| ATOM | 5093 | O | HOH | W 181 | 3.737   | 42.980 | 66.727 | 1.00 | 18.45 |
| ATOM | 5094 | O | HOH | W 182 | 10.657  | 69.135 | 86.850 | 1.00 | 30.21 |
| ATOM | 5095 | O | HOH | W 183 | 23.612  | 39.959 | 68.861 | 1.00 | 20.99 |
| ATOM | 5096 | O | HOH | W 184 | 30.240  | 50.378 | 93.511 | 1.00 | 31.76 |
| ATOM | 5097 | O | HOH | W 185 | 24.407  | 42.363 | 69.680 | 1.00 | 23.63 |
| ATOM | 5    |   |     |       |         |        |        |      |       |



|      |      |   |     |   |     |        |        |        |      |       |
|------|------|---|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 5115 | O | HOH | W | 203 | 8.373  | 35.496 | 71.320 | 1.00 | 34.46 |
| ATOM | 5116 | O | HOH | W | 204 | 30.102 | 60.104 | 96.117 | 1.00 | 23.15 |
| ATOM | 5117 | O | HOH | W | 205 | 28.927 | 39.455 | 66.453 | 1.00 | 21.12 |
| ATOM | 5118 | O | HOH | W | 206 | 39.689 | 41.335 | 88.297 | 1.00 | 27.24 |
| ATOM | 5119 | O | HOH | W | 207 | 33.916 | 37.626 | 52.438 | 1.00 | 33.19 |
| ATOM | 5120 | O | HOH | W | 208 | 1.622  | 50.963 | 82.588 | 1.00 | 50.35 |
| ATOM | 5121 | O | HOH | W | 209 | 16.333 | 60.146 | 56.900 | 1.00 | 29.60 |
| ATOM | 5122 | O | HOH | W | 210 | 39.242 | 45.128 | 91.725 | 1.00 | 22.90 |
| ATOM | 5123 | O | HOH | W | 211 | 14.399 | 30.418 | 45.430 | 1.00 | 34.78 |
| ATOM | 5124 | O | HOH | W | 212 | 29.888 | 42.111 | 88.891 | 1.00 | 34.76 |
| ATOM | 5125 | O | HOH | W | 213 | 18.346 | 26.212 | 50.297 | 1.00 | 44.2  |
| ATOM | 5126 | O | HOH | W | 214 | 22.864 | 63.026 | 74.711 | 1.00 | 29.30 |
| ATOM | 5127 | O | HOH | W | 215 | 20.113 | 37.220 | 85.926 | 1.00 | 24.06 |
| ATOM | 5128 | O | HOH | W | 216 | 23.298 | 70.540 | 87.208 | 1.00 | 35.89 |
| ATOM | 5129 | O | HOH | W | 217 | 26.970 | 41.872 | 69.933 | 1.00 | 28.60 |
| ATOM | 5130 | O | HOH | W | 218 | -4.296 | 44.927 | 43.216 | 1.00 | 33.90 |
| ATOM | 5131 | O | HOH | W | 219 | 12.321 | 60.082 | 62.828 | 1.00 | 28.33 |
| ATOM | 5132 | O | HOH | W | 220 | 13.873 | 37.878 | 45.419 | 1.00 | 43.55 |
| ATOM | 5133 | O | HOH | W | 221 | 30.748 | 40.180 | 83.791 | 1.00 | 37.04 |
| ATOM | 5134 | O | HOH | W | 222 | 15.784 | 58.732 | 93.087 | 1.00 | 23.80 |
| ATOM | 5135 | O | HOH | W | 223 | 35.311 | 18.767 | 63.462 | 1.00 | 49.24 |
| ATOM | 5136 | O | HOH | W | 224 | -0.325 | 33.536 | 77.400 | 1.00 | 28.59 |
| ATOM | 5137 | O | HOH | W | 225 | 9.312  | 60.280 | 65.861 | 1.00 | 37.85 |
| ATOM | 5138 | O | HOH | W | 226 | 20.424 | 20.146 | 83.661 | 1.00 | 32.68 |
| ATOM | 5139 | O | HOH | W | 227 | 10.879 | 65.256 | 88.761 | 1.00 | 28.17 |
| ATOM | 5140 | O | HOH | W | 228 | 6.481  | 11.890 | 66.154 | 1.00 | 13.58 |
| ATOM | 5141 | O | HOH | W | 229 | 11.493 | 12.304 | 65.667 | 1.00 | 31.38 |
| ATOM | 5142 | O | HOH | W | 230 | 23.893 | 48.760 | 67.764 | 1.00 | 19.58 |
| ATOM | 5143 | O | HOH | W | 231 | 11.826 | 33.465 | 74.498 | 1.00 | 16.87 |
| ATOM | 5144 | O | HOH | W | 232 | 20.228 | 48.799 | 84.083 | 1.00 | 14.10 |
| ATOM | 5145 | O | HOH | W | 233 | 8.333  | 25.989 | 83.238 | 1.00 | 20.03 |
| ATOM | 5146 | O | HOH | W | 234 | 24.244 | 65.422 | 90.512 | 1.00 | 18.61 |
| ATOM | 5147 | O | HOH | W | 235 | 29.682 | 43.395 | 86.674 | 1.00 | 29.99 |
| ATOM | 5148 | O | HOH | W | 236 | 32.122 | 38.935 | 81.421 | 1.00 | 21.98 |
| ATOM | 5149 | O | HOH | W | 237 | 38.098 | 44.260 | 70.626 | 1.00 | 23.18 |
| ATOM | 5150 | O | HOH | W | 238 | 17.172 | 68.773 | 81.829 | 1.00 | 33.19 |
| ATOM | 5151 | O | HOH | W | 239 | 22.056 | 41.676 | 85.707 | 1.00 | 27.98 |
| ATOM | 5152 | O | HOH | W | 240 | 10.609 | 35.835 | 76.035 | 1.00 | 26.77 |
| ATOM | 5153 | O | HOH | W | 241 | 5.895  | 48.362 | 80.563 | 1.00 | 35.27 |
| ATOM | 5154 | O | HOH | W | 242 | 4.210  | 38.365 | 90.354 | 1.00 | 62.63 |
| ATOM | 5155 | O | HOH | W | 243 | 27.505 | 26.048 | 57.570 | 1.00 | 34.59 |
| ATOM | 5156 | O | HOH | W | 244 | 40.199 | 29.895 | 75.610 | 1.00 | 30.81 |
| ATOM | 5157 | O | HOH |   |     |        |        |        |      |       |



66320-072703

|      |      |   |           |         |        |        |      |       |
|------|------|---|-----------|---------|--------|--------|------|-------|
| ATOM | 5176 | O | HOH W 264 | 0.397   | 52.925 | 76.187 | 1.00 | 26.73 |
| ATOM | 5177 | O | HOH W 265 | 24.642  | 68.564 | 81.573 | 1.00 | 27.40 |
| ATOM | 5178 | O | HOH W 266 | 25.734  | 20.393 | 55.492 | 1.00 | 32.87 |
| ATOM | 5179 | O | HOH W 267 | 11.923  | 58.720 | 70.763 | 1.00 | 21.77 |
| ATOM | 5180 | O | HOH W 268 | 30.308  | 43.013 | 67.201 | 1.00 | 35.32 |
| ATOM | 5181 | O | HOH W 269 | 39.640  | 38.126 | 67.437 | 1.00 | 28.94 |
| ATOM | 5182 | O | HOH W 270 | 10.397  | 50.110 | 41.557 | 1.00 | 28.07 |
| ATOM | 5183 | O | HOH W 271 | 33.290  | 46.466 | 61.539 | 1.00 | 27.30 |
| ATOM | 5184 | O | HOH W 272 | 0.016   | 42.090 | 76.502 | 1.00 | 32.33 |
| ATOM | 5185 | O | HOH W 273 | 26.563  | 45.481 | 40.291 | 1.00 | 47.85 |
| ATOM | 5186 | O | HOH W 274 | 30.451  | 15.205 | 70.110 | 1.00 | 33.04 |
| ATOM | 5187 | O | HOH W 275 | 0.678   | 54.618 | 69.973 | 1.00 | 30.37 |
| ATOM | 5188 | O | HOH W 276 | 31.009  | 22.826 | 58.292 | 1.00 | 38.03 |
| ATOM | 5189 | O | HOH W 277 | 11.598  | 18.077 | 78.103 | 1.00 | 32.86 |
| ATOM | 5190 | O | HOH W 278 | 42.789  | 49.257 | 82.276 | 1.00 | 38.27 |
| ATOM | 5191 | O | HOH W 279 | 22.610  | 37.483 | 44.945 | 1.00 | 36.88 |
| ATOM | 5192 | O | HOH W 280 | 19.095  | 19.104 | 54.480 | 1.00 | 29.52 |
| ATOM | 5193 | O | HOH W 281 | -17.217 | 39.695 | 36.067 | 1.00 | 33.38 |
| ATOM | 5194 | O | HOH W 282 | 6.068   | 42.637 | 67.543 | 1.00 | 33.87 |
| ATOM | 5195 | O | HOH W 283 | 20.639  | 46.522 | 87.847 | 1.00 | 36.70 |
| ATOM | 5196 | O | HOH W 284 | -8.870  | 56.242 | 58.240 | 1.00 | 50.62 |
| ATOM | 5197 | O | HOH W 285 | 16.582  | 61.670 | 59.151 | 1.00 | 38.20 |
| ATOM | 5198 | O | HOH W 286 | 42.501  | 43.301 | 75.886 | 1.00 | 27.81 |
| ATOM | 5199 | O | HOH W 287 | 25.604  | 33.439 | 84.786 | 1.00 | 21.08 |
| ATOM | 5200 | O | HOH W 288 | 13.520  | 67.352 | 52.561 | 1.00 | 39.75 |
| ATOM | 5201 | O | HOH W 289 | 9.627   | 28.198 | 45.908 | 1.00 | 37.35 |
| ATOM | 5202 | O | HOH W 290 | 18.134  | 36.512 | 88.493 | 1.00 | 43.01 |
| ATOM | 5203 | O | HOH W 291 | 22.300  | 20.482 | 81.874 | 1.00 | 37.81 |
| ATOM | 5204 | O | HOH W 292 | 44.203  | 41.289 | 79.602 | 1.00 | 27.00 |
| ATOM | 5205 | O | HOH W 293 | 44.462  | 52.335 | 93.395 | 1.00 | 32.88 |
| ATOM | 5206 | O | HOH W 294 | -2.968  | 37.813 | 43.815 | 1.00 | 39.42 |
| ATOM | 5207 | O | HOH W 295 | 14.615  | 50.638 | 83.483 | 1.00 | 40.84 |
| ATOM | 5208 | O | HOH W 296 | 17.655  | 48.236 | 85.049 | 1.00 | 38.41 |
| ATOM | 5209 | O | HOH W 297 | 25.105  | 58.534 | 70.338 | 1.00 | 45.37 |
| ATOM | 5210 | O | HOH W 298 | 6.153   | 22.174 | 58.465 | 1.00 | 51.17 |
| ATOM | 5211 | O | HOH W 299 | 14.099  | 45.045 | 75.129 | 1.00 | 38.12 |
| ATOM | 5212 | O | HOH W 300 | 3.614   | 33.798 | 78.265 | 1.00 | 33.77 |
| ATOM | 5213 | O | HOH W 301 | 10.974  | 62.101 | 70.086 | 1.00 | 31.30 |
| ATOM | 5214 | O | HOH W 302 | 7.585   | 38.532 | 71.479 | 1.00 | 35.66 |
| ATOM | 5215 | O | HOH W 303 | 20.998  | 44.178 | 74.359 | 1.00 | 37.38 |
| ATOM | 5216 | O | HOH W 304 | 11.918  | 38.385 | 43.252 | 1.00 | 35.61 |
| ATOM | 5217 | O | HOH W 305 | 34.337  | 29.948 | 80.309 | 1.00 | 36.78 |
| ATOM | 5218 | O | HOH W 306 | 39.120  | 63.630 | 75.316 | 1.00 | 43.48 |
| ATOM | 5219 | O | HOH W 307 | 36.491  | 64.702 | 80.717 | 1.00 | 19.64 |
| ATOM | 5220 | O | HOH W 308 | -11.598 | 58.968 | 55.040 | 1.00 | 54.59 |
| ATOM | 5221 | O | HOH W 309 | 18.873  | 53.508 | 93.447 | 1.00 | 29.42 |
| ATOM | 5222 | O | HOH W 310 | 7.673   | 37.412 | 69.273 | 1.00 | 30.92 |
| ATOM | 5223 | O | HOH W 311 | 38.494  | 29.355 | 71.433 | 1.00 | 35.92 |
| ATOM | 5224 | O | HOH W 312 | 2.378   | 64.614 | 72.106 | 1.00 | 23.68 |
| ATOM | 5225 | O | HOH W 313 | 34.055  | 22.747 | 70.419 | 1.00 | 47.42 |
| ATOM | 5226 | O | HOH W 314 | 6.517   | 15.338 | 63.891 | 1.00 | 39.21 |
| ATOM | 5227 | O | HOH W 315 | 33.135  | 58.667 | 95.357 | 1.00 | 38.27 |
| ATOM | 5228 | O | HOH W 316 | 7.877   | 41.088 | 68.810 | 1.00 | 30.88 |
| ATOM | 5229 | O | HOH W 317 | 4.500   | 63.686 | 62.465 | 1.00 | 40.54 |
| ATOM | 5230 | O | HOH W 318 | 32.594  | 44.212 | 51.619 | 1.00 | 28.18 |
| ATOM | 5231 | O | HOH W 319 | 19.892  | 28.363 | 50.295 | 1.00 | 37.48 |
| ATOM | 5232 | O | HOH W 320 | 38.121  | 42.209 | 58.482 | 1.00 | 35.42 |
| ATOM | 5233 | O | HOH W 321 | 18.953  | 60.209 | 59.879 | 1.00 | 32.37 |
| ATOM | 5234 | O | HOH W 322 | -1.038  | 45.854 | 73.695 | 1.00 | 33.19 |
| ATOM | 5235 | O | HOH W 323 | -6.723  | 31.695 | 78.229 | 1.00 | 48.52 |
| ATOM | 5236 | O | HOH W 324 | 20.123  | 41.413 | 71.190 | 1.00 | 40.23 |



5012240 022209

|      |      |   |     |   |     |         |        |        |      |       |
|------|------|---|-----|---|-----|---------|--------|--------|------|-------|
| ATOM | 5237 | O | HOH | W | 325 | 5.380   | 25.588 | 55.751 | 1.00 | 26.30 |
| ATOM | 5238 | O | HOH | W | 326 | -8.946  | 53.154 | 58.636 | 1.00 | 33.33 |
| ATOM | 5239 | O | HOH | W | 327 | 5.224   | 20.615 | 65.617 | 1.00 | 38.04 |
| ATOM | 5240 | O | HOH | W | 328 | -0.951  | 44.688 | 66.660 | 1.00 | 48.71 |
| ATOM | 5241 | O | HOH | W | 329 | 9.548   | 17.972 | 61.116 | 1.00 | 38.57 |
| ATOM | 5242 | O | HOH | W | 330 | 16.170  | 45.478 | 46.564 | 1.00 | 33.55 |
| ATOM | 5243 | O | HOH | W | 331 | 28.152  | 31.228 | 86.919 | 1.00 | 66.11 |
| ATOM | 5244 | O | HOH | W | 332 | -4.227  | 32.608 | 61.396 | 1.00 | 29.03 |
| ATOM | 5245 | O | HOH | W | 333 | 23.532  | 69.913 | 79.399 | 1.00 | 40.45 |
| ATOM | 5246 | O | HOH | W | 334 | 16.943  | 25.394 | 84.026 | 1.00 | 35.64 |
| ATOM | 5247 | O | HOH | W | 335 | -6.097  | 33.164 | 72.143 | 1.00 | 47.23 |
| ATOM | 5248 | O | HOH | W | 336 | 26.639  | 58.545 | 95.902 | 1.00 | 30.17 |
| ATOM | 5249 | O | HOH | W | 337 | 18.090  | 14.281 | 77.183 | 1.00 | 34.77 |
| ATOM | 5250 | O | HOH | W | 338 | 16.783  | 69.158 | 79.498 | 1.00 | 41.04 |
| ATOM | 5251 | O | HOH | W | 339 | 44.586  | 50.422 | 83.945 | 1.00 | 37.92 |
| ATOM | 5252 | O | HOH | W | 340 | 11.828  | 51.361 | 43.560 | 1.00 | 42.10 |
| ATOM | 5253 | O | HOH | W | 341 | 22.773  | 36.745 | 86.817 | 1.00 | 38.07 |
| ATOM | 5254 | O | HOH | W | 342 | 26.608  | 43.969 | 74.943 | 1.00 | 32.64 |
| ATOM | 5255 | O | HOH | W | 343 | 14.797  | 17.437 | 79.901 | 1.00 | 37.80 |
| ATOM | 5256 | O | HOH | W | 344 | 32.755  | 40.414 | 86.886 | 1.00 | 53.20 |
| ATOM | 5257 | O | HOH | W | 345 | 23.938  | 65.851 | 93.231 | 1.00 | 38.25 |
| ATOM | 5258 | O | HOH | W | 346 | 34.689  | 68.947 | 70.635 | 1.00 | 32.36 |
| ATOM | 5259 | O | HOH | W | 347 | 32.902  | 14.779 | 66.467 | 1.00 | 55.05 |
| ATOM | 5260 | O | HOH | W | 348 | -0.197  | 59.892 | 61.918 | 1.00 | 41.09 |
| ATOM | 5261 | O | HOH | W | 349 | 35.933  | 50.743 | 66.825 | 1.00 | 29.14 |
| ATOM | 5262 | O | HOH | W | 350 | 21.451  | 70.196 | 84.069 | 1.00 | 37.63 |
| ATOM | 5263 | O | HOH | W | 351 | 10.392  | 34.055 | 71.909 | 1.00 | 37.36 |
| ATOM | 5264 | O | HOH | W | 352 | 16.118  | 48.288 | 46.594 | 1.00 | 33.56 |
| ATOM | 5265 | O | HOH | W | 353 | 2.277   | 58.481 | 67.819 | 1.00 | 45.09 |
| ATOM | 5266 | O | HOH | W | 354 | -21.140 | 42.970 | 52.987 | 1.00 | 38.49 |
| ATOM | 5267 | O | HOH | W | 355 | 0.364   | 56.797 | 65.209 | 1.00 | 34.76 |
| ATOM | 5268 | O | HOH | W | 356 | 9.763   | 37.511 | 72.464 | 1.00 | 36.84 |
| ATOM | 5269 | O | HOH | W | 357 | -3.293  | 29.651 | 64.159 | 1.00 | 48.44 |
| ATOM | 5270 | O | HOH | W | 358 | 18.653  | 59.497 | 55.820 | 1.00 | 41.32 |
| ATOM | 5271 | O | HOH | W | 359 | 18.360  | 56.858 | 89.365 | 1.00 | 16.20 |
| ATOM | 5272 | O | HOH | W | 360 | 19.264  | 58.334 | 58.324 | 1.00 | 24.32 |
| ATOM | 5273 | O | HOH | W | 361 | 19.786  | 68.920 | 85.535 | 1.00 | 36.46 |
| ATOM | 5274 | O | HOH | W | 362 | 0.891   | 46.454 | 70.028 | 1.00 | 49.40 |
| ATOM | 5275 | O | HOH | W | 363 | 13.401  | 15.156 | 61.247 | 1.00 | 32.90 |
| ATOM | 5276 | O | HOH | W | 364 | 29.937  | 41.912 | 73.484 | 1.00 | 34.92 |
| ATOM | 5277 | O | HOH | W | 365 | 28.117  | 39.053 | 82.612 | 1.00 | 29.94 |
| ATOM | 5278 | O | HOH | W | 366 | 17.060  | 44.064 | 76.687 | 1.00 | 31.64 |
| ATOM | 5279 | O | HOH | W | 367 | 7.781   | 32.331 | 42.244 | 1.00 | 54.33 |
| ATOM | 5280 | O | HOH | W | 368 | 13.484  | 60.143 | 67.092 | 1.00 | 36.32 |
| ATOM | 5281 | O | HOH | W | 369 | 4.972   | 65.695 | 69.472 | 1.00 | 30.93 |
| ATOM | 5282 | O | HOH | W | 370 | 20.859  | 55.364 | 94.926 | 1.00 | 35.05 |
| ATOM | 5283 | O | HOH | W | 371 | 29.891  | 64.316 | 94.062 | 1.00 | 32.43 |
| ATOM | 5284 | O | HOH | W | 372 | 31.636  | 50.857 | 46.407 | 1.00 | 75.60 |
| ATOM | 5285 | O | HOH | W | 373 | -9.778  | 35.027 | 39.632 | 1.00 | 56.74 |
| ATOM | 5286 | O | HOH | W | 374 | 14.152  | 12.701 | 64.957 | 1.00 | 23.80 |
| ATOM | 5287 | O | HOH | W | 375 | 35.419  | 45.143 | 64.442 | 1.00 | 36.74 |
| ATOM | 5288 | O | HOH | W | 376 | 34.839  | 57.375 | 97.888 | 1.00 | 34.34 |
| ATOM | 5289 | O | HOH | W | 377 | 35.027  | 44.946 | 53.379 | 1.00 | 45.25 |
| ATOM | 5290 | O | HOH | W | 378 | 10.904  | 44.942 | 78.238 | 1.00 | 46.33 |
| ATOM | 5291 | O | HOH | W | 379 | 2.265   | 29.749 | 79.673 | 1.00 | 55.34 |
| ATOM | 5292 | O | HOH | W | 380 | 38.376  | 37.663 | 83.485 | 1.00 | 48.83 |
| ATOM | 5293 | O | HOH | W | 381 | 7.069   | 18.511 | 64.588 | 1.00 | 42.75 |
| ATOM | 5294 | O | HOH | W | 382 | 10.013  | 63.184 | 65.119 | 1.00 | 51.27 |
| ATOM | 5295 | O | HOH | W | 383 | 26.880  | 67.265 | 80.460 | 1.00 | 29.17 |
| ATOM | 5296 | O | HOH | W | 384 | 5.435   | 44.858 | 39.529 | 1.00 | 44.09 |
| ATOM | 5297 | O | HOH | W | 385 | 12.020  | 76.116 | 49.503 | 1.00 | 57.08 |



66920 072209

|      |      |   |           |         |        |        |      |       |
|------|------|---|-----------|---------|--------|--------|------|-------|
| ATOM | 5298 | O | HOH W 386 | 4.495   | 69.223 | 72.134 | 1.00 | 39.49 |
| ATOM | 5299 | O | HOH W 387 | 34.373  | 34.834 | 52.407 | 1.00 | 45.73 |
| ATOM | 5300 | O | HOH W 388 | -0.366  | 52.210 | 68.045 | 1.00 | 56.86 |
| ATOM | 5301 | O | HOH W 389 | 15.108  | 39.899 | 89.165 | 1.00 | 30.62 |
| ATOM | 5302 | O | HOH W 390 | 20.977  | 60.725 | 61.985 | 1.00 | 42.08 |
| ATOM | 5303 | O | HOH W 391 | 29.038  | 14.547 | 63.725 | 1.00 | 33.69 |
| ATOM | 5304 | O | HOH W 392 | 34.064  | 66.637 | 81.988 | 1.00 | 37.83 |
| ATOM | 5305 | O | HOH W 393 | 8.669   | 71.915 | 54.348 | 1.00 | 40.01 |
| ATOM | 5306 | O | HOH W 394 | 4.823   | 29.577 | 79.259 | 1.00 | 42.09 |
| ATOM | 5307 | O | HOH W 395 | 22.745  | 32.929 | 42.078 | 1.00 | 50.18 |
| ATOM | 5308 | O | HOH W 396 | 0.658   | 29.749 | 51.236 | 1.00 | 30.86 |
| ATOM | 5309 | O | HOH W 397 | 3.793   | 58.214 | 86.346 | 1.00 | 62.42 |
| ATOM | 5310 | O | HOH W 398 | 12.206  | 40.564 | 89.850 | 1.00 | 39.66 |
| ATOM | 5311 | O | HOH W 399 | 21.573  | 25.561 | 53.053 | 1.00 | 34.62 |
| ATOM | 5312 | O | HOH W 400 | 30.197  | 56.551 | 58.739 | 1.00 | 40.16 |
| ATOM | 5313 | O | HOH W 401 | 20.406  | 59.350 | 64.941 | 1.00 | 33.97 |
| ATOM | 5314 | O | HOH W 402 | 16.956  | 52.960 | 87.724 | 1.00 | 54.35 |
| ATOM | 5315 | O | HOH W 403 | 36.719  | 27.459 | 68.822 | 1.00 | 42.51 |
| ATOM | 5316 | O | HOH W 404 | 7.458   | 27.206 | 77.481 | 1.00 | 46.67 |
| ATOM | 5317 | O | HOH W 405 | 36.220  | 64.298 | 90.593 | 1.00 | 51.29 |
| ATOM | 5318 | O | HOH W 406 | -17.985 | 43.406 | 48.900 | 1.00 | 41.71 |
| ATOM | 5319 | O | HOH W 407 | 1.914   | 29.246 | 53.120 | 1.00 | 38.28 |
| ATOM | 5320 | O | HOH W 408 | -4.267  | 29.328 | 73.970 | 1.00 | 34.50 |
| ATOM | 5321 | O | HOH W 409 | 14.000  | 53.360 | 42.218 | 1.00 | 42.56 |
| ATOM | 5322 | O | HOH W 410 | 5.615   | 22.345 | 61.668 | 1.00 | 59.03 |
| ATOM | 5323 | O | HOH W 411 | -3.455  | 50.442 | 63.951 | 1.00 | 44.90 |
| ATOM | 5324 | O | HOH W 412 | 29.002  | 38.811 | 44.563 | 1.00 | 43.27 |
| ATOM | 5325 | O | HOH W 413 | 37.416  | 55.208 | 61.603 | 1.00 | 42.90 |
| ATOM | 5326 | O | HOH W 414 | 14.459  | 14.960 | 73.514 | 1.00 | 42.33 |
| ATOM | 5327 | O | HOH W 415 | 35.076  | 48.768 | 98.233 | 1.00 | 41.69 |
| ATOM | 5328 | O | HOH W 416 | 6.452   | 56.342 | 86.263 | 1.00 | 34.79 |
| ATOM | 5329 | O | HOH W 417 | 35.573  | 17.694 | 66.735 | 1.00 | 40.65 |
| ATOM | 5330 | O | HOH W 418 | 28.756  | 59.314 | 74.937 | 1.00 | 35.85 |
| ATOM | 5331 | O | HOH W 419 | 12.955  | 64.913 | 53.664 | 1.00 | 37.44 |
| ATOM | 5332 | O | HOH W 420 | 23.309  | 24.474 | 50.751 | 1.00 | 45.73 |
| ATOM | 5333 | O | HOH W 421 | 4.924   | 27.771 | 55.010 | 1.00 | 38.46 |
| ATOM | 5334 | O | HOH W 422 | 19.668  | 63.675 | 93.111 | 1.00 | 41.69 |
| ATOM | 5335 | O | HOH W 423 | 29.343  | 46.551 | 40.650 | 1.00 | 45.12 |
| ATOM | 5336 | O | HOH W 424 | 28.230  | 48.770 | 60.385 | 1.00 | 40.19 |
| ATOM | 5337 | O | HOH W 425 | 14.292  | 23.244 | 85.078 | 1.00 | 32.92 |
| ATOM | 5338 | O | HOH W 426 | 7.179   | 66.298 | 48.617 | 1.00 | 47.43 |
| ATOM | 5339 | O | HOH W 427 | -11.542 | 35.315 | 64.224 | 1.00 | 45.74 |
| ATOM | 5340 | O | HOH W 428 | -0.665  | 52.874 | 80.688 | 1.00 | 44.47 |
| ATOM | 5341 | O | HOH W 429 | -1.483  | 67.437 | 44.508 | 1.00 | 88.79 |
| ATOM | 5342 | O | HOH W 430 | 13.367  | 66.767 | 63.127 | 1.00 | 62.36 |
| ATOM | 5343 | O | HOH W 431 | 35.060  | 48.549 | 63.034 | 1.00 | 39.85 |
| ATOM | 5344 | O | HOH W 432 | 11.721  | 60.705 | 42.372 | 1.00 | 56.11 |
| ATOM | 5345 | O | HOH W 433 | 14.261  | 27.588 | 85.980 | 1.00 | 51.35 |
| ATOM | 5346 | O | HOH W 434 | 38.915  | 34.680 | 61.103 | 1.00 | 45.58 |
| ATOM | 5347 | O | HOH W 435 | 23.421  | 46.416 | 42.605 | 1.00 | 43.02 |
| ATOM | 5348 | O | HOH W 436 | 19.154  | 28.435 | 86.238 | 1.00 | 47.30 |
| ATOM | 5349 | O | HOH W 437 | 26.658  | 43.571 | 47.275 | 1.00 | 34.55 |
| ATOM | 5350 | O | HOH W 438 | 15.725  | 45.758 | 43.317 | 1.00 | 43.06 |
| ATOM | 5351 | O | HOH W 439 | 36.546  | 66.825 | 82.882 | 1.00 | 30.83 |
| ATOM | 5352 | O | HOH W 440 | 8.498   | 74.001 | 52.039 | 1.00 | 46.91 |
| ATOM | 5353 | O | HOH W 441 | 27.161  | 71.692 | 92.146 | 1.00 | 39.00 |
| ATOM | 5354 | O | HOH W 442 | 27.946  | 33.322 | 85.163 | 1.00 | 33.09 |
| ATOM | 5355 | O | HOH W 443 | 15.310  | 10.169 | 65.089 | 1.00 | 63.51 |
| ATOM | 5356 | O | HOH W 444 | -13.474 | 41.923 | 71.321 | 1.00 | 44.29 |
| ATOM | 5357 | O | HOH W 445 | -6.593  | 61.419 | 56.587 | 1.00 | 36.57 |
| ATOM | 5358 | O | HOH W 446 | -4.107  | 19.122 | 50.753 | 1.00 | 80.39 |



60122110-022599

|      |      |   |           |         |        |         |      |       |
|------|------|---|-----------|---------|--------|---------|------|-------|
| ATOM | 5359 | O | HOH W 447 | 21.809  | 59.754 | 43.571  | 1.00 | 64.03 |
| ATOM | 5360 | O | HOH W 448 | 32.503  | 55.926 | 51.478  | 1.00 | 51.13 |
| ATOM | 5361 | O | HOH W 449 | 17.433  | 44.251 | 80.196  | 1.00 | 52.95 |
| ATOM | 5362 | O | HOH W 450 | -2.882  | 28.319 | 76.738  | 1.00 | 57.32 |
| ATOM | 5363 | O | HOH W 451 | 8.921   | 18.143 | 71.756  | 1.00 | 45.59 |
| ATOM | 5364 | O | HOH W 452 | 46.415  | 37.408 | 72.673  | 1.00 | 74.61 |
| ATOM | 5365 | O | HOH W 453 | 46.612  | 53.365 | 82.940  | 1.00 | 41.92 |
| ATOM | 5366 | O | HOH W 454 | 39.885  | 53.691 | 74.043  | 1.00 | 45.59 |
| ATOM | 5367 | O | HOH W 455 | 28.187  | 69.890 | 80.215  | 1.00 | 33.51 |
| ATOM | 5368 | O | HOH W 456 | 10.557  | 47.292 | 72.599  | 1.00 | 14.04 |
| ATOM | 5369 | O | HOH W 457 | -0.687  | 61.537 | 70.644  | 1.00 | 40.63 |
| ATOM | 5370 | O | HOH W 458 | 33.335  | 31.445 | 62.420  | 1.00 | 32.53 |
| ATOM | 5371 | O | HOH W 459 | 26.658  | 39.474 | 43.256  | 1.00 | 32.50 |
| ATOM | 5372 | O | HOH W 460 | 30.185  | 25.893 | 82.542  | 1.00 | 45.40 |
| ATOM | 5373 | O | HOH W 461 | 20.780  | 39.620 | 40.793  | 1.00 | 60.63 |
| ATOM | 5374 | O | HOH W 462 | -13.804 | 40.073 | 67.421  | 1.00 | 42.25 |
| ATOM | 5375 | O | HOH W 463 | 1.328   | 41.371 | 78.681  | 1.00 | 56.39 |
| ATOM | 5376 | O | HOH W 464 | 33.554  | 26.796 | 70.488  | 1.00 | 37.48 |
| ATOM | 5377 | O | HOH W 465 | 34.317  | 54.835 | 70.139  | 1.00 | 57.37 |
| ATOM | 5378 | O | HOH W 466 | 1.781   | 11.779 | 66.821  | 1.00 | 47.25 |
| ATOM | 5379 | O | HOH W 467 | 13.278  | 63.141 | 46.031  | 1.00 | 57.79 |
| ATOM | 5380 | O | HOH W 468 | 37.787  | 55.035 | 100.999 | 1.00 | 53.08 |
| ATOM | 5381 | O | HOH W 469 | 13.794  | 19.603 | 83.707  | 1.00 | 47.87 |
| ATOM | 5382 | O | HOH W 470 | 25.470  | 45.716 | 93.468  | 1.00 | 36.66 |
| ATOM | 5383 | O | HOH W 471 | 10.578  | 17.685 | 75.291  | 1.00 | 37.43 |
| ATOM | 5384 | O | HOH W 472 | 52.811  | 39.642 | 69.739  | 1.00 | 44.12 |
| ATOM | 5385 | O | HOH W 473 | 23.329  | 56.116 | 94.868  | 1.00 | 47.73 |
| ATOM | 5386 | O | HOH W 474 | 35.936  | 48.711 | 65.428  | 1.00 | 58.05 |
| ATOM | 5387 | O | HOH W 475 | 28.119  | 66.507 | 82.635  | 1.00 | 41.75 |
| ATOM | 5388 | O | HOH W 476 | -0.565  | 54.408 | 74.299  | 1.00 | 50.86 |
| ATOM | 5389 | O | HOH W 477 | 4.072   | 70.416 | 58.486  | 1.00 | 35.45 |
| ATOM | 5390 | O | HOH W 478 | -3.762  | 26.579 | 63.779  | 1.00 | 53.91 |
| ATOM | 5391 | O | HOH W 479 | 19.595  | 35.426 | 41.883  | 1.00 | 51.58 |
| ATOM | 5392 | O | HOH W 480 | 24.800  | 7.578  | 70.043  | 1.00 | 41.13 |
| ATOM | 5393 | O | HOH W 481 | 17.947  | 10.147 | 65.643  | 1.00 | 58.35 |
| ATOM | 5394 | O | HOH W 482 | 31.312  | 44.348 | 64.437  | 1.00 | 48.49 |
| ATOM | 5395 | O | HOH W 483 | 46.224  | 50.030 | 81.043  | 1.00 | 53.87 |
| ATOM | 5396 | O | HOH W 484 | 35.129  | 52.464 | 51.431  | 1.00 | 54.76 |
| ATOM | 5397 | O | HOH W 485 | 5.885   | 65.189 | 84.813  | 1.00 | 83.91 |
| ATOM | 5398 | O | HOH W 486 | 20.281  | 16.200 | 55.863  | 1.00 | 46.25 |
| ATOM | 5399 | O | HOH W 487 | -5.180  | 21.053 | 56.028  | 1.00 | 37.00 |
| ATOM | 5400 | O | HOH W 488 | -11.188 | 38.067 | 41.229  | 1.00 | 69.22 |
| ATOM | 5401 | O | HOH W 489 | 15.256  | 67.180 | 75.313  | 1.00 | 51.22 |
| ATOM | 5402 | O | HOH W 490 | 3.374   | 63.019 | 56.672  | 1.00 | 42.46 |
| ATOM | 5403 | O | HOH W 491 | 30.082  | 15.975 | 73.952  | 1.00 | 49.06 |
| ATOM | 5404 | O | HOH W 492 | -7.562  | 32.348 | 64.350  | 1.00 | 53.88 |
| ATOM | 5405 | O | HOH W 493 | 14.504  | 69.382 | 77.201  | 1.00 | 79.52 |
| ATOM | 5406 | O | HOH W 494 | 37.374  | 41.179 | 54.837  | 1.00 | 41.94 |
| ATOM | 5407 | O | HOH W 495 | 22.651  | 62.725 | 71.998  | 1.00 | 46.62 |
| ATOM | 5408 | O | HOH W 496 | 13.052  | 47.941 | 46.569  | 1.00 | 50.14 |
| ATOM | 5409 | O | HOH W 497 | -1.906  | 45.997 | 36.480  | 1.00 | 62.33 |
| ATOM | 5410 | O | HOH W 498 | 35.740  | 52.464 | 53.693  | 1.00 | 55.17 |
| ATOM | 5411 | O | HOH W 499 | 30.727  | 32.353 | 49.843  | 1.00 | 56.92 |
| ATOM | 5412 | O | HOH W 500 | 0.025   | 32.686 | 42.604  | 1.00 | 48.23 |
| ATOM | 5413 | O | HOH W 501 | 47.830  | 56.735 | 86.611  | 1.00 | 47.42 |
| ATOM | 5414 | O | HOH W 502 | 18.095  | 60.627 | 94.715  | 1.00 | 65.28 |
| ATOM | 5415 | O | HOH W 503 | 2.306   | 31.026 | 81.802  | 1.00 | 37.32 |
| ATOM | 5416 | O | HOH W 504 | -8.696  | 27.990 | 79.237  | 1.00 | 46.99 |
| ATOM | 5417 | O | HOH W 505 | 22.034  | 70.217 | 89.142  | 1.00 | 47.15 |
| ATOM | 5418 | O | HOH W 506 | 22.136  | 73.412 | 87.005  | 1.00 | 38.47 |
| ATOM | 5419 | O | HOH W 507 | -0.926  | 26.674 | 74.129  | 1.00 | 58.76 |



|      |      |   |           |         |        |        |      |        |
|------|------|---|-----------|---------|--------|--------|------|--------|
| ATOM | 5420 | O | HOH W 508 | -6.108  | 48.377 | 71.102 | 1.00 | 64.56  |
| ATOM | 5421 | O | HOH W 509 | 39.520  | 39.424 | 56.576 | 1.00 | 72.80  |
| ATOM | 5422 | O | HOH W 510 | -4.081  | 58.518 | 47.377 | 1.00 | 60.65  |
| ATOM | 5423 | O | HOH W 511 | 34.434  | 23.876 | 75.179 | 1.00 | 48.53  |
| ATOM | 5424 | O | HOH W 512 | 17.400  | 63.380 | 50.267 | 1.00 | 40.76  |
| ATOM | 5425 | O | HOH W 513 | 9.647   | 61.533 | 68.296 | 1.00 | 46.31  |
| ATOM | 5426 | O | HOH W 514 | 41.430  | 58.961 | 99.800 | 1.00 | 49.23  |
| ATOM | 5427 | O | HOH W 515 | 23.725  | 20.340 | 53.830 | 1.00 | 51.65  |
| ATOM | 5428 | O | HOH W 516 | 15.576  | 16.190 | 78.131 | 1.00 | 61.27  |
| ATOM | 5429 | O | HOH W 517 | 29.334  | 21.375 | 75.882 | 1.00 | 44.80  |
| ATOM | 5430 | O | HOH W 518 | -1.624  | 50.514 | 39.683 | 1.00 | 49.85  |
| ATOM | 5431 | O | HOH W 519 | 8.771   | 69.104 | 72.705 | 1.00 | 47.81  |
| ATOM | 5432 | O | HOH W 520 | -21.311 | 45.001 | 55.217 | 1.00 | 64.01  |
| ATOM | 5433 | O | HOH W 521 | -1.392  | 54.790 | 67.171 | 1.00 | 53.90  |
| ATOM | 5434 | O | HOH W 522 | 38.464  | 56.277 | 74.548 | 1.00 | 63.93  |
| ATOM | 5435 | O | HOH W 523 | 33.977  | 32.491 | 81.832 | 1.00 | 50.18  |
| ATOM | 5436 | O | HOH W 524 | 16.060  | 54.317 | 91.714 | 1.00 | 61.57  |
| ATOM | 5437 | O | HOH W 525 | 21.009  | 33.700 | 89.176 | 1.00 | 65.31  |
| ATOM | 5438 | O | HOH W 526 | 28.726  | 36.253 | 85.146 | 1.00 | 34.76  |
| ATOM | 5439 | O | HOH W 527 | 24.767  | 40.641 | 41.912 | 1.00 | 44.57  |
| ATOM | 5440 | O | HOH W 528 | 40.708  | 69.261 | 83.251 | 1.00 | 39.08  |
| ATOM | 5441 | O | HOH W 529 | 28.264  | 48.404 | 92.814 | 1.00 | 34.64  |
| ATOM | 5442 | O | HOH W 530 | 19.375  | 61.177 | 66.689 | 1.00 | 44.16  |
| ATOM | 5443 | O | HOH W 531 | 6.639   | 42.598 | 82.079 | 1.00 | 100.00 |
| ATOM | 5444 | O | HOH W 532 | 40.403  | 33.306 | 64.502 | 1.00 | 45.36  |
| ATOM | 5445 | O | HOH W 533 | 16.172  | 18.117 | 52.264 | 1.00 | 44.76  |
| ATOM | 5446 | O | HOH W 534 | 33.899  | 42.310 | 48.851 | 1.00 | 52.28  |
| ATOM | 5447 | O | HOH W 535 | 22.675  | 9.894  | 76.942 | 1.00 | 51.28  |
| ATOM | 5448 | O | HOH W 536 | -11.295 | 52.730 | 60.674 | 1.00 | 76.16  |
| ATOM | 5449 | O | HOH W 537 | 20.605  | 66.466 | 58.378 | 1.00 | 61.62  |
| ATOM | 5450 | O | HOH W 538 | 35.282  | 26.341 | 50.576 | 1.00 | 58.72  |
| ATOM | 5451 | O | HOH W 539 | -0.234  | 39.225 | 40.255 | 1.00 | 54.13  |
| ATOM | 5452 | O | HOH W 540 | 36.597  | 43.931 | 57.481 | 1.00 | 43.52  |
| ATOM | 5453 | O | HOH W 541 | 20.374  | 41.951 | 74.120 | 1.00 | 47.12  |
| ATOM | 5454 | O | HOH W 542 | 31.857  | 31.721 | 82.689 | 1.00 | 46.66  |
| ATOM | 5455 | O | HOH W 543 | 34.733  | 63.213 | 92.164 | 1.00 | 55.58  |
| ATOM | 5456 | O | HOH W 544 | -20.506 | 26.471 | 44.860 | 1.00 | 73.89  |
| ATOM | 5457 | O | HOH W 545 | 37.699  | 32.453 | 62.558 | 1.00 | 46.00  |
| ATOM | 5458 | O | HOH W 546 | 8.296   | 38.910 | 67.642 | 1.00 | 39.42  |
| ATOM | 5459 | O | HOH W 547 | 0.194   | 69.671 | 72.188 | 1.00 | 47.07  |
| ATOM | 5460 | O | HOH W 548 | 32.212  | 52.268 | 51.134 | 1.00 | 52.82  |
| ATOM | 5461 | O | HOH W 549 | 33.917  | 21.004 | 64.439 | 1.00 | 26.12  |
| ATOM | 5462 | O | HOH W 550 | 42.573  | 58.916 | 95.252 | 1.00 | 20.78  |
| ATOM | 5463 | O | HOH W 551 | 34.529  | 66.786 | 72.611 | 1.00 | 36.24  |



Table 10: Structure coordinates of LTA<sub>4</sub> hydrolase-thiolamine complex

|        |                     |         |         |        |        |         |              |
|--------|---------------------|---------|---------|--------|--------|---------|--------------|
| CRYST  | 68.560              | 132.150 | 83.270  | 90.00  | 90.00  | 90.00   | P21212       |
| SCALE1 | 0.01459             | 0.00000 | 0.00000 |        |        | 0.00000 |              |
| SCALE2 | 0.00000             | 0.00757 | 0.00000 |        |        | 0.00000 |              |
| SCALE3 | 0.00000             | 0.00000 | 0.01201 |        |        | 0.00000 |              |
|        |                     |         |         |        |        |         |              |
|        | Atom res. Chain No. |         |         | x      | y      | z       | occ B-factor |
| ATOM   | 1                   | N       | PRO A 1 | -0.593 | 16.387 | 63.494  | 1.00 97.99   |
| ATOM   | 2                   | CA      | PRO A 1 | -1.890 | 16.918 | 63.874  | 1.00 97.22   |
| ATOM   | 3                   | C       | PRO A 1 | -2.210 | 18.371 | 63.525  | 1.00100.00   |
| ATOM   | 4                   | O       | PRO A 1 | -2.402 | 18.667 | 62.342  | 1.00100.00   |
| ATOM   | 5                   | CB      | PRO A 1 | -2.130 | 16.551 | 65.332  | 1.00 97.81   |
| ATOM   | 6                   | CG      | PRO A 1 | -1.221 | 15.355 | 65.583  | 1.00100.00   |
| ATOM   | 7                   | CD      | PRO A 1 | -0.290 | 15.233 | 64.369  | 1.00 97.05   |
| ATOM   | 8                   | N       | GLU A 2 | -2.216 | 19.272 | 64.556  | 1.00 96.95   |
| ATOM   | 9                   | CA      | GLU A 2 | -2.569 | 20.678 | 64.314  | 1.00 95.71   |
| ATOM   | 10                  | C       | GLU A 2 | -2.188 | 21.701 | 65.386  | 1.00 94.33   |
| ATOM   | 11                  | O       | GLU A 2 | -2.512 | 21.542 | 66.562  | 1.00 93.21   |
| ATOM   | 12                  | CB      | GLU A 2 | -4.105 | 20.768 | 64.214  | 1.00 97.26   |
| ATOM   | 13                  | CG      | GLU A 2 | -4.587 | 21.732 | 63.125  | 1.00100.00   |
| ATOM   | 14                  | CD      | GLU A 2 | -4.351 | 21.139 | 61.767  | 1.00100.00   |
| ATOM   | 15                  | OE1     | GLU A 2 | -3.301 | 21.261 | 61.152  | 1.00100.00   |
| ATOM   | 16                  | OE2     | GLU A 2 | -5.361 | 20.398 | 61.368  | 1.00100.00   |
| ATOM   | 17                  | N       | ILE A 3 | -1.550 | 22.799 | 64.944  | 1.00 86.29   |
| ATOM   | 18                  | CA      | ILE A 3 | -1.148 | 23.905 | 65.820  | 1.00 81.53   |
| ATOM   | 19                  | C       | ILE A 3 | -2.006 | 25.154 | 65.661  | 1.00 75.68   |
| ATOM   | 20                  | O       | ILE A 3 | -2.835 | 25.288 | 64.763  | 1.00 76.97   |
| ATOM   | 21                  | CB      | ILE A 3 | 0.308  | 24.324 | 65.707  | 1.00 83.45   |
| ATOM   | 22                  | CG1     | ILE A 3 | 0.452  | 25.521 | 64.759  | 1.00 83.63   |
| ATOM   | 23                  | CG2     | ILE A 3 | 1.198  | 23.160 | 65.300  | 1.00 84.76   |
| ATOM   | 24                  | CD1     | ILE A 3 | -0.184 | 25.361 | 63.375  | 1.00 91.36   |
| ATOM   | 25                  | N       | VAL A 4 | -1.725 | 26.099 | 66.523  | 1.00 61.54   |
| ATOM   | 26                  | CA      | VAL A 4 | -2.477 | 27.303 | 66.482  | 1.00 56.32   |
| ATOM   | 27                  | C       | VAL A 4 | -1.658 | 28.552 | 66.623  | 1.00 50.98   |
| ATOM   | 28                  | O       | VAL A 4 | -0.803 | 28.694 | 67.512  | 1.00 47.84   |
| ATOM   | 29                  | CB      | VAL A 4 | -3.514 | 27.318 | 67.595  | 1.00 58.99   |
| ATOM   | 30                  | CG1     | VAL A 4 | -3.735 | 28.754 | 68.047  | 1.00 58.40   |
| ATOM   | 31                  | CG2     | VAL A 4 | -4.819 | 26.691 | 67.131  | 1.00 58.56   |
| ATOM   | 32                  | N       | ASP A 5 | -2.012 | 29.486 | 65.732  | 1.00 39.38   |
| ATOM   | 33                  | CA      | ASP A 5 | -1.403 | 30.782 | 65.763  | 1.00 32.64   |
| ATOM   | 34                  | C       | ASP A 5 | -2.308 | 31.596 | 66.634  | 1.00 36.35   |
| ATOM   | 35                  | O       | ASP A 5 | -3.343 | 32.051 | 66.171  | 1.00 38.30   |
| ATOM   | 36                  | CB      | ASP A 5 | -1.252 | 31.492 | 64.400  | 1.00 30.79   |
| ATOM   | 37                  | CG      | ASP A 5 | -0.251 | 32.581 | 64.563  | 1.00 29.96   |
| ATOM   | 38                  | OD1     | ASP A 5 | -0.069 | 33.123 | 65.635  | 1.00 35.01   |
| ATOM   | 39                  | OD2     | ASP A 5 | 0.457  | 32.831 | 63.493  | 1.00 29.81   |
| ATOM   | 40                  | N       | THR A 6 | -1.931 | 31.745 | 67.903  | 1.00 32.32   |
| ATOM   | 41                  | CA      | THR A 6 | -2.710 | 32.507 | 68.842  | 1.00 32.08   |
| ATOM   | 42                  | C       | THR A 6 | -2.701 | 34.011 | 68.557  | 1.00 40.63   |
| ATOM   | 43                  | O       | THR A 6 | -3.484 | 34.759 | 69.132  | 1.00 46.68   |
| ATOM   | 44                  | CB      | THR A 6 | -2.357 | 32.171 | 70.295  | 1.00 44.71   |
| ATOM   | 45                  | OG1     | THR A 6 | -0.967 | 32.322 | 70.505  | 1.00 51.05   |
| ATOM   | 46                  | CG2     | THR A 6 | -2.789 | 30.741 | 70.604  | 1.00 35.79   |
| ATOM   | 47                  | N       | CYS A 7 | -1.842 | 34.480 | 67.656  | 1.00 32.51   |
| ATOM   | 48                  | CA      | CYS A 7 | -1.797 | 35.923 | 67.335  | 1.00 28.92   |
| ATOM   | 49                  | C       | CYS A 7 | -2.627 | 36.329 | 66.129  | 1.00 31.49   |
| ATOM   | 50                  | O       | CYS A 7 | -2.780 | 37.523 | 65.875  | 1.00 25.42   |
| ATOM   | 51                  | CB      | CYS A 7 | -0.362 | 36.410 | 67.107  | 1.00 27.38   |



|      |    |     |     |   |    |         |        |        |      |       |
|------|----|-----|-----|---|----|---------|--------|--------|------|-------|
| ATOM | 52 | SG  | CYS | A | 7  | 0.686   | 35.944 | 68.518 | 1.00 | 32.02 |
| ATOM | 53 | N   | SER | A | 8  | -3.140  | 35.315 | 65.383 | 1.00 | 34.03 |
| ATOM | 54 | CA  | SER | A | 8  | -3.940  | 35.508 | 64.158 | 1.00 | 32.97 |
| ATOM | 55 | C   | SER | A | 8  | -5.410  | 35.136 | 64.264 | 1.00 | 33.52 |
| ATOM | 56 | O   | SER | A | 8  | -5.744  | 34.137 | 64.866 | 1.00 | 32.89 |
| ATOM | 57 | CB  | SER | A | 8  | -3.363  | 34.754 | 62.980 | 1.00 | 34.07 |
| ATOM | 58 | OG  | SER | A | 8  | -4.017  | 35.182 | 61.798 | 1.00 | 36.65 |
| ATOM | 59 | N   | LEU | A | 9  | -6.289  | 35.921 | 63.635 | 1.00 | 30.79 |
| ATOM | 60 | CA  | LEU | A | 9  | -7.724  | 35.649 | 63.672 | 1.00 | 31.91 |
| ATOM | 61 | C   | LEU | A | 9  | -8.198  | 35.009 | 62.377 | 1.00 | 36.07 |
| ATOM | 62 | O   | LEU | A | 9  | -9.359  | 34.626 | 62.216 | 1.00 | 38.67 |
| ATOM | 63 | CB  | LEU | A | 9  | -8.514  | 36.958 | 63.874 | 1.00 | 32.47 |
| ATOM | 64 | CG  | LEU | A | 9  | -8.306  | 37.688 | 65.212 | 1.00 | 35.39 |
| ATOM | 65 | CD1 | LEU | A | 9  | -9.113  | 38.983 | 65.193 | 1.00 | 32.27 |
| ATOM | 66 | CD2 | LEU | A | 9  | -8.746  | 36.816 | 66.397 | 1.00 | 33.25 |
| ATOM | 67 | N   | ALA | A | 10 | -7.273  | 34.933 | 61.443 | 1.00 | 28.63 |
| ATOM | 68 | CA  | ALA | A | 10 | -7.545  | 34.408 | 60.147 | 1.00 | 27.14 |
| ATOM | 69 | C   | ALA | A | 10 | -7.643  | 32.921 | 60.090 | 1.00 | 34.34 |
| ATOM | 70 | O   | ALA | A | 10 | -7.296  | 32.173 | 61.005 | 1.00 | 37.34 |
| ATOM | 71 | CB  | ALA | A | 10 | -6.551  | 34.936 | 59.100 | 1.00 | 27.72 |
| ATOM | 72 | N   | SER | A | 11 | -8.130  | 32.503 | 58.959 | 1.00 | 32.08 |
| ATOM | 73 | CA  | SER | A | 11 | -8.256  | 31.115 | 58.708 | 1.00 | 32.03 |
| ATOM | 74 | C   | SER | A | 11 | -6.838  | 30.519 | 58.656 | 1.00 | 32.67 |
| ATOM | 75 | O   | SER | A | 11 | -5.927  | 31.028 | 57.986 | 1.00 | 29.29 |
| ATOM | 76 | CB  | SER | A | 11 | -9.013  | 30.934 | 57.401 | 1.00 | 38.42 |
| ATOM | 77 | OG  | SER | A | 11 | -10.391 | 30.728 | 57.648 | 1.00 | 44.17 |
| ATOM | 78 | N   | PRO | A | 12 | -6.651  | 29.440 | 59.387 | 1.00 | 29.14 |
| ATOM | 79 | CA  | PRO | A | 12 | -5.370  | 28.786 | 59.476 | 1.00 | 26.83 |
| ATOM | 80 | C   | PRO | A | 12 | -4.935  | 28.176 | 58.173 | 1.00 | 32.64 |
| ATOM | 81 | O   | PRO | A | 12 | -5.737  | 28.007 | 57.284 | 1.00 | 35.89 |
| ATOM | 82 | CB  | PRO | A | 12 | -5.544  | 27.698 | 60.540 | 1.00 | 28.28 |
| ATOM | 83 | CG  | PRO | A | 12 | -7.029  | 27.571 | 60.843 | 1.00 | 32.92 |
| ATOM | 84 | CD  | PRO | A | 12 | -7.731  | 28.587 | 59.952 | 1.00 | 30.42 |
| ATOM | 85 | N   | ALA | A | 13 | -3.645  | 27.836 | 58.063 | 1.00 | 30.63 |
| ATOM | 86 | CA  | ALA | A | 13 | -3.066  | 27.236 | 56.855 | 1.00 | 28.36 |
| ATOM | 87 | C   | ALA | A | 13 | -3.644  | 25.852 | 56.576 | 1.00 | 33.99 |
| ATOM | 88 | O   | ALA | A | 13 | -3.455  | 25.240 | 55.528 | 1.00 | 31.60 |
| ATOM | 89 | CB  | ALA | A | 13 | -1.561  | 27.133 | 57.050 | 1.00 | 27.68 |
| ATOM | 90 | N   | SER | A | 14 | -4.338  | 25.352 | 57.571 | 1.00 | 31.10 |
| ATOM | 91 | CA  | SER | A | 14 | -4.919  | 24.069 | 57.469 | 1.00 | 30.66 |
| ATOM | 92 | C   | SER | A | 14 | -6.242  | 24.133 | 56.753 | 1.00 | 37.86 |
| ATOM | 93 | O   | SER | A | 14 | -6.768  | 23.118 | 56.328 | 1.00 | 45.79 |
| ATOM | 94 | CB  | SER | A | 14 | -5.005  | 23.386 | 58.825 | 1.00 | 34.33 |
| ATOM | 95 | OG  | SER | A | 14 | -6.006  | 23.978 | 59.621 | 1.00 | 41.01 |
| ATOM | 96 | N   | VAL | A | 15 | -6.785  | 25.327 | 56.630 |      |       |



|      |     |     |     |   |    |        |        |        |      |       |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|
| ATOM | 113 | CB  | ARG | A | 17 | -2.371 | 28.152 | 51.758 | 1.00 | 36.83 |
| ATOM | 114 | CG  | ARG | A | 17 | -1.779 | 27.391 | 52.915 | 1.00 | 40.61 |
| ATOM | 115 | CD  | ARG | A | 17 | -1.472 | 25.970 | 52.503 | 1.00 | 27.18 |
| ATOM | 116 | NE  | ARG | A | 17 | -1.963 | 25.026 | 53.501 | 1.00 | 52.41 |
| ATOM | 117 | CZ  | ARG | A | 17 | -1.244 | 24.036 | 54.035 | 1.00 | 69.41 |
| ATOM | 118 | NH1 | ARG | A | 17 | 0.020  | 23.812 | 53.683 | 1.00 | 54.86 |
| ATOM | 119 | NH2 | ARG | A | 17 | -1.810 | 23.246 | 54.952 | 1.00 | 49.68 |
| ATOM | 120 | N   | THR | A | 18 | -2.711 | 31.454 | 51.378 | 1.00 | 27.06 |
| ATOM | 121 | CA  | THR | A | 18 | -2.489 | 32.477 | 50.428 | 1.00 | 26.12 |
| ATOM | 122 | C   | THR | A | 18 | -1.250 | 32.110 | 49.653 | 1.00 | 30.83 |
| ATOM | 123 | O   | THR | A | 18 | -0.174 | 31.964 | 50.194 | 1.00 | 29.06 |
| ATOM | 124 | CB  | THR | A | 18 | -2.276 | 33.810 | 51.134 | 1.00 | 34.27 |
| ATOM | 125 | OG1 | THR | A | 18 | -3.481 | 34.261 | 51.738 | 1.00 | 32.95 |
| ATOM | 126 | CG2 | THR | A | 18 | -1.730 | 34.839 | 50.156 | 1.00 | 35.91 |
| ATOM | 127 | N   | LYS | A | 19 | -1.408 | 31.955 | 48.365 | 1.00 | 31.55 |
| ATOM | 128 | CA  | LYS | A | 19 | -0.298 | 31.615 | 47.511 | 1.00 | 31.74 |
| ATOM | 129 | C   | LYS | A | 19 | 0.359  | 32.848 | 46.906 | 1.00 | 33.90 |
| ATOM | 130 | O   | LYS | A | 19 | 1.513  | 32.834 | 46.520 | 1.00 | 34.57 |
| ATOM | 131 | CB  | LYS | A | 19 | -0.795 | 30.697 | 46.398 | 1.00 | 36.08 |
| ATOM | 132 | CG  | LYS | A | 19 | -1.332 | 29.368 | 46.924 | 1.00 | 62.54 |
| ATOM | 133 | CD  | LYS | A | 19 | -0.281 | 28.257 | 47.057 | 1.00 | 82.23 |
| ATOM | 134 | CE  | LYS | A | 19 | 0.093  | 27.880 | 48.496 | 1.00 | 77.50 |
| ATOM | 135 | NZ  | LYS | A | 19 | 1.553  | 27.849 | 48.745 | 1.00 | 55.63 |
| ATOM | 136 | N   | HIS | A | 20 | -0.387 | 33.928 | 46.810 | 1.00 | 31.40 |
| ATOM | 137 | CA  | HIS | A | 20 | 0.160  | 35.122 | 46.198 | 1.00 | 29.22 |
| ATOM | 138 | C   | HIS | A | 20 | -0.655 | 36.345 | 46.517 | 1.00 | 34.68 |
| ATOM | 139 | O   | HIS | A | 20 | -1.833 | 36.239 | 46.846 | 1.00 | 35.34 |
| ATOM | 140 | CB  | HIS | A | 20 | 0.123  | 34.956 | 44.666 | 1.00 | 26.47 |
| ATOM | 141 | CG  | HIS | A | 20 | 0.865  | 36.022 | 43.970 | 1.00 | 26.77 |
| ATOM | 142 | ND1 | HIS | A | 20 | 2.249  | 36.046 | 43.980 | 1.00 | 28.92 |
| ATOM | 143 | CD2 | HIS | A | 20 | 0.415  | 37.091 | 43.280 | 1.00 | 27.43 |
| ATOM | 144 | CE1 | HIS | A | 20 | 2.622  | 37.126 | 43.301 | 1.00 | 28.21 |
| ATOM | 145 | NE2 | HIS | A | 20 | 1.536  | 37.781 | 42.865 | 1.00 | 28.18 |
| ATOM | 146 | N   | LEU | A | 21 | 0.000  | 37.492 | 46.390 | 1.00 | 30.14 |
| ATOM | 147 | CA  | LEU | A | 21 | -0.596 | 38.782 | 46.610 | 1.00 | 31.02 |
| ATOM | 148 | C   | LEU | A | 21 | -0.134 | 39.786 | 45.562 | 1.00 | 38.34 |
| ATOM | 149 | O   | LEU | A | 21 | 1.073  | 39.952 | 45.312 | 1.00 | 37.30 |
| ATOM | 150 | CB  | LEU | A | 21 | -0.342 | 39.363 | 47.999 | 1.00 | 31.30 |
| ATOM | 151 | CG  | LEU | A | 21 | -0.611 | 40.880 | 48.047 | 1.00 | 32.33 |
| ATOM | 152 | CD1 | LEU | A | 21 | -2.088 | 41.192 | 48.324 | 1.00 | 27.10 |
| ATOM | 153 | CD2 | LEU | A | 21 | 0.277  | 41.522 | 49.100 | 1.00 | 32.86 |
| ATOM | 154 | N   | HIS | A | 22 | -1.127 | 40.442 | 44.951 | 1.00 | 35.47 |
| ATOM | 155 | CA  | HIS | A | 22 | -0.895 | 41.452 | 43.920 | 1.00 | 34.24 |
| ATOM | 156 | C   | HIS | A | 22 | -1.249 | 42.742 | 44.550 | 1.00 |       |



|      |     |     |     |   |    |        |        |        |      |        |
|------|-----|-----|-----|---|----|--------|--------|--------|------|--------|
| ATOM | 174 | C   | ARG | A | 24 | -1.930 | 49.005 | 44.562 | 1.00 | 39.15  |
| ATOM | 175 | O   | ARG | A | 24 | -3.025 | 48.859 | 45.107 | 1.00 | 39.85  |
| ATOM | 176 | CB  | ARG | A | 24 | -2.458 | 47.716 | 42.504 | 1.00 | 46.35  |
| ATOM | 177 | CG  | ARG | A | 24 | -2.054 | 46.750 | 41.382 | 1.00 | 50.50  |
| ATOM | 178 | CD  | ARG | A | 24 | -2.754 | 47.058 | 40.043 | 1.00 | 80.27  |
| ATOM | 179 | NE  | ARG | A | 24 | -4.200 | 46.798 | 40.062 | 1.00 | 95.12  |
| ATOM | 180 | CZ  | ARG | A | 24 | -5.152 | 47.703 | 39.826 | 1.00 | 100.00 |
| ATOM | 181 | NH1 | ARG | A | 24 | -4.863 | 48.973 | 39.483 | 1.00 | 100.00 |
| ATOM | 182 | NH2 | ARG | A | 24 | -6.432 | 47.326 | 39.865 | 1.00 | 100.00 |
| ATOM | 183 | N   | CYS | A | 25 | -1.164 | 50.028 | 44.844 | 1.00 | 32.39  |
| ATOM | 184 | CA  | CYS | A | 25 | -1.698 | 50.969 | 45.813 | 1.00 | 33.30  |
| ATOM | 185 | C   | CYS | A | 25 | -1.061 | 52.325 | 45.724 | 1.00 | 34.82  |
| ATOM | 186 | O   | CYS | A | 25 | -0.012 | 52.514 | 45.076 | 1.00 | 31.03  |
| ATOM | 187 | CB  | CYS | A | 25 | -1.503 | 50.440 | 47.257 | 1.00 | 34.67  |
| ATOM | 188 | SG  | CYS | A | 25 | 0.231  | 50.529 | 47.798 | 1.00 | 38.07  |
| ATOM | 189 | N   | SER | A | 26 | -1.711 | 53.257 | 46.418 | 1.00 | 34.39  |
| ATOM | 190 | CA  | SER | A | 26 | -1.196 | 54.601 | 46.437 | 1.00 | 36.77  |
| ATOM | 191 | C   | SER | A | 26 | -0.963 | 55.133 | 47.821 | 1.00 | 39.85  |
| ATOM | 192 | O   | SER | A | 26 | -1.738 | 54.853 | 48.757 | 1.00 | 37.56  |
| ATOM | 193 | CB  | SER | A | 26 | -1.889 | 55.600 | 45.530 | 1.00 | 42.70  |
| ATOM | 194 | OG  | SER | A | 26 | -0.899 | 56.330 | 44.824 | 1.00 | 61.74  |
| ATOM | 195 | N   | VAL | A | 27 | 0.133  | 55.897 | 47.886 | 1.00 | 39.43  |
| ATOM | 196 | CA  | VAL | A | 27 | 0.624  | 56.583 | 49.081 | 1.00 | 41.31  |
| ATOM | 197 | C   | VAL | A | 27 | 0.209  | 58.043 | 49.082 | 1.00 | 44.32  |
| ATOM | 198 | O   | VAL | A | 27 | 0.562  | 58.799 | 48.187 | 1.00 | 45.24  |
| ATOM | 199 | CB  | VAL | A | 27 | 2.135  | 56.531 | 49.207 | 1.00 | 46.35  |
| ATOM | 200 | CG1 | VAL | A | 27 | 2.524  | 57.207 | 50.522 | 1.00 | 45.62  |
| ATOM | 201 | CG2 | VAL | A | 27 | 2.592  | 55.079 | 49.178 | 1.00 | 47.20  |
| ATOM | 202 | N   | ASP | A | 28 | -0.553 | 58.417 | 50.093 | 1.00 | 37.94  |
| ATOM | 203 | CA  | ASP | A | 28 | -1.040 | 59.764 | 50.237 | 1.00 | 35.28  |
| ATOM | 204 | C   | ASP | A | 28 | -0.595 | 60.366 | 51.538 | 1.00 | 33.85  |
| ATOM | 205 | O   | ASP | A | 28 | -1.181 | 60.099 | 52.598 | 1.00 | 28.52  |
| ATOM | 206 | CB  | ASP | A | 28 | -2.559 | 59.807 | 50.189 | 1.00 | 37.09  |
| ATOM | 207 | CG  | ASP | A | 28 | -3.055 | 61.205 | 50.095 | 1.00 | 55.20  |
| ATOM | 208 | OD1 | ASP | A | 28 | -2.611 | 62.119 | 50.767 | 1.00 | 59.17  |
| ATOM | 209 | OD2 | ASP | A | 28 | -3.993 | 61.335 | 49.192 | 1.00 | 61.41  |
| ATOM | 210 | N   | PHE | A | 29 | 0.436  | 61.174 | 51.405 | 1.00 | 36.42  |
| ATOM | 211 | CA  | PHE | A | 29 | 1.044  | 61.888 | 52.512 | 1.00 | 43.07  |
| ATOM | 212 | C   | PHE | A | 29 | 0.105  | 62.928 | 53.077 | 1.00 | 51.14  |
| ATOM | 213 | O   | PHE | A | 29 | 0.161  | 63.279 | 54.257 | 1.00 | 51.35  |
| ATOM | 214 | CB  | PHE | A | 29 | 2.410  | 62.517 | 52.143 | 1.00 | 47.77  |
| ATOM | 215 | CG  | PHE | A | 29 | 3.519  | 61.485 | 52.079 | 1.00 | 50.86  |
| ATOM | 216 | CD1 | PHE | A | 29 | 4.066  | 60.957 | 53.247 | 1.00 | 52.08  |
| ATOM | 217 | CD2 | PHE | A | 29 | 3.996  | 61.001 | 50.863 | 1.00 | 53.94  |
| ATOM |     |     |     |   |    |        |        |        |      |        |



60123410-022699

|      |     |     |     |   |    |        |        |        |            |
|------|-----|-----|-----|---|----|--------|--------|--------|------------|
| ATOM | 235 | NE  | ARG | A | 31 | -7.344 | 60.450 | 50.327 | 1.00100.00 |
| ATOM | 236 | CZ  | ARG | A | 31 | -8.148 | 60.371 | 49.251 | 1.00100.00 |
| ATOM | 237 | NH1 | ARG | A | 31 | -9.034 | 61.324 | 48.944 | 1.00100.00 |
| ATOM | 238 | NH2 | ARG | A | 31 | -8.062 | 59.298 | 48.460 | 1.00100.00 |
| ATOM | 239 | N   | ARG | A | 32 | -2.489 | 60.752 | 54.683 | 1.00 39.71 |
| ATOM | 240 | CA  | ARG | A | 32 | -1.751 | 59.798 | 55.531 | 1.00 39.09 |
| ATOM | 241 | C   | ARG | A | 32 | -2.324 | 58.411 | 55.379 | 1.00 39.62 |
| ATOM | 242 | O   | ARG | A | 32 | -2.495 | 57.655 | 56.337 | 1.00 33.10 |
| ATOM | 243 | CB  | ARG | A | 32 | -1.523 | 60.115 | 57.022 | 1.00 37.14 |
| ATOM | 244 | CG  | ARG | A | 32 | -1.197 | 61.569 | 57.337 | 1.00 71.25 |
| ATOM | 245 | CD  | ARG | A | 32 | 0.277  | 61.834 | 57.686 | 1.00100.00 |
| ATOM | 246 | NE  | ARG | A | 32 | 0.703  | 61.299 | 58.986 | 1.00100.00 |
| ATOM | 247 | CZ  | ARG | A | 32 | 1.284  | 62.005 | 59.961 | 1.00 79.51 |
| ATOM | 248 | NH1 | ARG | A | 32 | 1.522  | 63.308 | 59.831 | 1.00 55.73 |
| ATOM | 249 | NH2 | ARG | A | 32 | 1.626  | 61.387 | 61.098 | 1.00 44.96 |
| ATOM | 250 | N   | THR | A | 33 | -2.612 | 58.068 | 54.139 | 1.00 39.83 |
| ATOM | 251 | CA  | THR | A | 33 | -3.162 | 56.752 | 53.902 | 1.00 39.31 |
| ATOM | 252 | C   | THR | A | 33 | -2.543 | 56.010 | 52.760 | 1.00 41.13 |
| ATOM | 253 | O   | THR | A | 33 | -1.853 | 56.574 | 51.926 | 1.00 42.93 |
| ATOM | 254 | CB  | THR | A | 33 | -4.635 | 56.835 | 53.641 | 1.00 43.44 |
| ATOM | 255 | OG1 | THR | A | 33 | -4.798 | 57.636 | 52.468 | 1.00 40.17 |
| ATOM | 256 | CG2 | THR | A | 33 | -5.245 | 57.468 | 54.880 | 1.00 38.71 |
| ATOM | 257 | N   | LEU | A | 34 | -2.822 | 54.717 | 52.762 | 1.00 35.26 |
| ATOM | 258 | CA  | LEU | A | 34 | -2.372 | 53.799 | 51.745 | 1.00 35.20 |
| ATOM | 259 | C   | LEU | A | 34 | -3.632 | 53.293 | 51.098 | 1.00 32.49 |
| ATOM | 260 | O   | LEU | A | 34 | -4.474 | 52.670 | 51.751 | 1.00 30.96 |
| ATOM | 261 | CB  | LEU | A | 34 | -1.522 | 52.651 | 52.322 | 1.00 37.07 |
| ATOM | 262 | CG  | LEU | A | 34 | -0.149 | 52.571 | 51.685 | 1.00 42.99 |
| ATOM | 263 | CD1 | LEU | A | 34 | 0.648  | 51.425 | 52.285 | 1.00 40.58 |
| ATOM | 264 | CD2 | LEU | A | 34 | -0.360 | 52.302 | 50.208 | 1.00 50.83 |
| ATOM | 265 | N   | THR | A | 35 | -3.800 | 53.632 | 49.838 | 1.00 28.72 |
| ATOM | 266 | CA  | THR | A | 35 | -5.017 | 53.228 | 49.198 | 1.00 31.26 |
| ATOM | 267 | C   | THR | A | 35 | -4.838 | 52.329 | 48.013 | 1.00 36.54 |
| ATOM | 268 | O   | THR | A | 35 | -3.940 | 52.546 | 47.187 | 1.00 34.70 |
| ATOM | 269 | CB  | THR | A | 35 | -5.877 | 54.427 | 48.813 | 1.00 44.88 |
| ATOM | 270 | OG1 | THR | A | 35 | -5.484 | 55.549 | 49.579 | 1.00 58.59 |
| ATOM | 271 | CG2 | THR | A | 35 | -7.324 | 54.094 | 49.109 | 1.00 49.42 |
| ATOM | 272 | N   | GLY | A | 36 | -5.726 | 51.329 | 47.950 | 1.00 32.57 |
| ATOM | 273 | CA  | GLY | A | 36 | -5.696 | 50.405 | 46.837 | 1.00 33.89 |
| ATOM | 274 | C   | GLY | A | 36 | -6.418 | 49.074 | 46.993 | 1.00 34.50 |
| ATOM | 275 | O   | GLY | A | 36 | -7.441 | 48.919 | 47.678 | 1.00 31.78 |
| ATOM | 276 | N   | THR | A | 37 | -5.836 | 48.103 | 46.293 | 1.00 35.93 |
| ATOM | 277 | CA  | THR | A | 37 | -6.327 | 46.723 | 46.281 | 1.00 36.12 |
| ATOM | 278 | C   | THR | A | 37 | -5.268 | 45.696 | 46.473 | 1.00 35.67 |
| ATOM | 279 | O   | THR | A | 37 | -4.155 | 45.795 | 45.964 | 1.00 33.86 |
| ATOM | 280 | CB  | THR | A | 37 | -7.119 | 46.306 | 45.050 | 1.00 42.21 |
| ATOM | 281 | OG1 | THR | A | 37 | -6.507 | 46.804 | 43.870 | 1.00 30.98 |
| ATOM | 282 | CG2 | THR | A | 37 | -8.547 | 46.793 | 45.229 | 1.00 50.03 |
| ATOM | 283 | N   | ALA | A | 38 | -5.687 | 44.705 | 47.220 | 1.00 32.95 |
| ATOM | 284 | CA  | ALA | A | 38 | -4.886 | 43.570 | 47.533 | 1.00 33.45 |
| ATOM | 285 | C   | ALA | A | 38 | -5.481 | 42.374 | 46.824 | 1.00 35.47 |
| ATOM | 286 | O   | ALA | A | 38 | -6.580 | 41.906 | 47.151 | 1.00 32.91 |
| ATOM | 287 | CB  | ALA | A | 38 | -4.845 | 43.341 | 49.044 | 1.00 33.72 |
| ATOM | 288 | N   | ALA | A | 39 | -4.764 | 41.874 | 45.834 | 1.00 32.70 |
| ATOM | 289 | CA  | ALA | A | 39 | -5.274 | 40.702 | 45.140 | 1.00 31.59 |
| ATOM | 290 | C   | ALA | A | 39 | -4.692 | 39.464 | 45.770 | 1.00 32.11 |
| ATOM | 291 | O   | ALA | A | 39 | -3.514 | 39.147 | 45.608 | 1.00 32.46 |
| ATOM | 292 | CB  | ALA | A | 39 | -4.934 | 40.729 | 43.662 | 1.00 32.13 |
| ATOM | 293 | N   | LEU | A | 40 | -5.505 | 38.774 | 46.508 | 1.00 27.06 |
| ATOM | 294 | CA  | LEU | A | 40 | -5.001 | 37.593 | 47.155 | 1.00 29.04 |
| ATOM | 295 | C   | LEU | A | 40 | -5.331 | 36.322 | 46.364 | 1.00 36.88 |



|      |     |     |     |   |    |         |        |        |      |       |
|------|-----|-----|-----|---|----|---------|--------|--------|------|-------|
| ATOM | 296 | O   | LEU | A | 40 | -6.485  | 36.100 | 45.963 | 1.00 | 28.89 |
| ATOM | 297 | CB  | LEU | A | 40 | -5.587  | 37.451 | 48.600 | 1.00 | 29.39 |
| ATOM | 298 | CG  | LEU | A | 40 | -5.303  | 38.598 | 49.559 | 1.00 | 31.39 |
| ATOM | 299 | CD1 | LEU | A | 40 | -5.435  | 38.063 | 50.970 | 1.00 | 32.62 |
| ATOM | 300 | CD2 | LEU | A | 40 | -3.879  | 39.019 | 49.355 | 1.00 | 31.60 |
| ATOM | 301 | N   | THR | A | 41 | -4.310  | 35.470 | 46.165 | 1.00 | 42.40 |
| ATOM | 302 | CA  | THR | A | 41 | -4.523  | 34.210 | 45.488 | 1.00 | 43.93 |
| ATOM | 303 | C   | THR | A | 41 | -4.548  | 33.155 | 46.552 | 1.00 | 43.75 |
| ATOM | 304 | O   | THR | A | 41 | -3.510  | 32.827 | 47.115 | 1.00 | 45.22 |
| ATOM | 305 | CB  | THR | A | 41 | -3.511  | 33.892 | 44.402 | 1.00 | 55.44 |
| ATOM | 306 | OG1 | THR | A | 41 | -3.604  | 34.885 | 43.418 | 1.00 | 55.57 |
| ATOM | 307 | CG2 | THR | A | 41 | -3.872  | 32.544 | 43.802 | 1.00 | 47.78 |
| ATOM | 308 | N   | VAL | A | 42 | -5.755  | 32.688 | 46.848 | 1.00 | 33.25 |
| ATOM | 309 | CA  | VAL | A | 42 | -5.946  | 31.720 | 47.893 | 1.00 | 32.21 |
| ATOM | 310 | C   | VAL | A | 42 | -6.166  | 30.312 | 47.380 | 1.00 | 40.56 |
| ATOM | 311 | O   | VAL | A | 42 | -6.827  | 30.105 | 46.376 | 1.00 | 42.56 |
| ATOM | 312 | CB  | VAL | A | 42 | -7.017  | 32.153 | 48.920 | 1.00 | 36.45 |
| ATOM | 313 | CG1 | VAL | A | 42 | -6.817  | 31.451 | 50.266 | 1.00 | 36.89 |
| ATOM | 314 | CG2 | VAL | A | 42 | -6.963  | 33.665 | 49.170 | 1.00 | 36.10 |
| ATOM | 315 | N   | GLN | A | 43 | -5.590  | 29.357 | 48.117 | 1.00 | 35.91 |
| ATOM | 316 | CA  | GLN | A | 43 | -5.678  | 27.945 | 47.838 | 1.00 | 31.59 |
| ATOM | 317 | C   | GLN | A | 43 | -6.346  | 27.244 | 48.988 | 1.00 | 38.98 |
| ATOM | 318 | O   | GLN | A | 43 | -5.916  | 27.317 | 50.144 | 1.00 | 40.92 |
| ATOM | 319 | CB  | GLN | A | 43 | -4.305  | 27.319 | 47.568 | 1.00 | 30.50 |
| ATOM | 320 | CG  | GLN | A | 43 | -4.362  | 25.800 | 47.259 | 1.00 | 53.80 |
| ATOM | 321 | CD  | GLN | A | 43 | -2.986  | 25.177 | 47.099 | 1.00 | 62.47 |
| ATOM | 322 | OE1 | GLN | A | 43 | -2.569  | 24.842 | 45.978 | 1.00 | 57.34 |
| ATOM | 323 | NE2 | GLN | A | 43 | -2.274  | 25.037 | 48.224 | 1.00 | 43.72 |
| ATOM | 324 | N   | SER | A | 44 | -7.423  | 26.555 | 48.664 | 1.00 | 33.83 |
| ATOM | 325 | CA  | SER | A | 44 | -8.166  | 25.839 | 49.678 | 1.00 | 31.38 |
| ATOM | 326 | C   | SER | A | 44 | -7.495  | 24.557 | 50.117 | 1.00 | 42.10 |
| ATOM | 327 | O   | SER | A | 44 | -6.955  | 23.814 | 49.292 | 1.00 | 42.78 |
| ATOM | 328 | CB  | SER | A | 44 | -9.576  | 25.530 | 49.226 | 1.00 | 28.60 |
| ATOM | 329 | OG  | SER | A | 44 | -10.234 | 24.785 | 50.224 | 1.00 | 34.57 |
| ATOM | 330 | N   | GLN | A | 45 | -7.579  | 24.286 | 51.423 | 1.00 | 38.84 |
| ATOM | 331 | CA  | GLN | A | 45 | -7.007  | 23.082 | 51.994 | 1.00 | 37.05 |
| ATOM | 332 | C   | GLN | A | 45 | -8.082  | 22.050 | 52.269 | 1.00 | 47.57 |
| ATOM | 333 | O   | GLN | A | 45 | -7.801  | 20.917 | 52.678 | 1.00 | 42.94 |
| ATOM | 334 | CB  | GLN | A | 45 | -6.247  | 23.411 | 53.280 | 1.00 | 36.10 |
| ATOM | 335 | CG  | GLN | A | 45 | -5.246  | 24.539 | 53.034 | 1.00 | 54.73 |
| ATOM | 336 | CD  | GLN | A | 45 | -4.323  | 24.206 | 51.888 | 1.00 | 45.43 |
| ATOM | 337 | OE1 | GLN | A | 45 | -4.257  | 24.888 | 50.833 | 1.00 | 39.23 |
| ATOM | 338 | NE2 | GLN | A | 45 | -3.621  | 23.121 | 52.092 | 1.00 | 29.80 |
| ATOM | 339 | N   | GLU | A | 46 | -9.330  | 22.459 | 52.048 | 1.0  |       |







|      |     |     |     |   |    |         |        |        |      |        |
|------|-----|-----|-----|---|----|---------|--------|--------|------|--------|
| ATOM | 375 | O   | ARG | A | 50 | -17.627 | 30.760 | 51.011 | 1.00 | 53.89  |
| ATOM | 376 | CB  | ARG | A | 50 | -18.928 | 28.028 | 51.986 | 1.00 | 58.35  |
| ATOM | 377 | CG  | ARG | A | 50 | -19.863 | 27.354 | 50.980 | 1.00 | 74.76  |
| ATOM | 378 | CD  | ARG | A | 50 | -20.438 | 26.024 | 51.462 | 1.00 | 81.60  |
| ATOM | 379 | NE  | ARG | A | 50 | -21.214 | 25.355 | 50.415 | 1.00 | 94.37  |
| ATOM | 380 | CZ  | ARG | A | 50 | -22.465 | 24.888 | 50.538 | 1.00 | 100.00 |
| ATOM | 381 | NH1 | ARG | A | 50 | -23.151 | 24.990 | 51.687 | 1.00 | 100.00 |
| ATOM | 382 | NH2 | ARG | A | 50 | -23.046 | 24.297 | 49.471 | 1.00 | 74.34  |
| ATOM | 383 | N   | SER | A | 51 | -16.331 | 30.006 | 52.743 | 1.00 | 54.71  |
| ATOM | 384 | CA  | SER | A | 51 | -15.823 | 31.297 | 53.224 | 1.00 | 53.49  |
| ATOM | 385 | C   | SER | A | 51 | -14.495 | 31.156 | 53.955 | 1.00 | 53.57  |
| ATOM | 386 | O   | SER | A | 51 | -14.146 | 30.062 | 54.420 | 1.00 | 52.93  |
| ATOM | 387 | CB  | SER | A | 51 | -16.788 | 31.900 | 54.232 | 1.00 | 54.03  |
| ATOM | 388 | OG  | SER | A | 51 | -16.871 | 31.048 | 55.373 | 1.00 | 45.15  |
| ATOM | 389 | N   | LEU | A | 52 | -13.796 | 32.298 | 54.067 | 1.00 | 47.19  |
| ATOM | 390 | CA  | LEU | A | 52 | -12.519 | 32.422 | 54.762 | 1.00 | 45.66  |
| ATOM | 391 | C   | LEU | A | 52 | -12.415 | 33.671 | 55.640 | 1.00 | 50.43  |
| ATOM | 392 | O   | LEU | A | 52 | -13.145 | 34.633 | 55.471 | 1.00 | 52.64  |
| ATOM | 393 | CB  | LEU | A | 52 | -11.235 | 32.117 | 53.923 | 1.00 | 44.20  |
| ATOM | 394 | CG  | LEU | A | 52 | -10.896 | 33.044 | 52.745 | 1.00 | 43.98  |
| ATOM | 395 | CD1 | LEU | A | 52 | -11.739 | 32.687 | 51.554 | 1.00 | 42.82  |
| ATOM | 396 | CD2 | LEU | A | 52 | -11.128 | 34.501 | 53.094 | 1.00 | 44.71  |
| ATOM | 397 | N   | VAL | A | 53 | -11.483 | 33.658 | 56.579 | 1.00 | 44.97  |
| ATOM | 398 | CA  | VAL | A | 53 | -11.271 | 34.781 | 57.455 | 1.00 | 41.69  |
| ATOM | 399 | C   | VAL | A | 53 | -9.859  | 35.309 | 57.339 | 1.00 | 44.25  |
| ATOM | 400 | O   | VAL | A | 53 | -8.866  | 34.551 | 57.302 | 1.00 | 45.42  |
| ATOM | 401 | CB  | VAL | A | 53 | -11.565 | 34.420 | 58.906 | 1.00 | 45.48  |
| ATOM | 402 | CG1 | VAL | A | 53 | -11.223 | 35.554 | 59.853 | 1.00 | 44.94  |
| ATOM | 403 | CG2 | VAL | A | 53 | -13.030 | 34.073 | 59.050 | 1.00 | 45.79  |
| ATOM | 404 | N   | LEU | A | 54 | -9.796  | 36.627 | 57.166 | 1.00 | 35.12  |
| ATOM | 405 | CA  | LEU | A | 54 | -8.555  | 37.333 | 57.080 | 1.00 | 34.14  |
| ATOM | 406 | C   | LEU | A | 54 | -8.377  | 38.207 | 58.326 | 1.00 | 38.92  |
| ATOM | 407 | O   | LEU | A | 54 | -9.281  | 38.457 | 59.108 | 1.00 | 37.45  |
| ATOM | 408 | CB  | LEU | A | 54 | -8.461  | 38.216 | 55.831 | 1.00 | 34.73  |
| ATOM | 409 | CG  | LEU | A | 54 | -8.539  | 37.469 | 54.510 | 1.00 | 40.25  |
| ATOM | 410 | CD1 | LEU | A | 54 | -8.416  | 38.488 | 53.374 | 1.00 | 40.69  |
| ATOM | 411 | CD2 | LEU | A | 54 | -7.424  | 36.428 | 54.415 | 1.00 | 39.64  |
| ATOM | 412 | N   | ASP | A | 55 | -7.192  | 38.674 | 58.524 | 1.00 | 35.02  |
| ATOM | 413 | CA  | ASP | A | 55 | -6.918  | 39.526 | 59.627 | 1.00 | 31.65  |
| ATOM | 414 | C   | ASP | A | 55 | -6.956  | 40.941 | 59.078 | 1.00 | 40.38  |
| ATOM | 415 | O   | ASP | A | 55 | -6.754  | 41.151 | 57.886 | 1.00 | 39.98  |
| ATOM | 416 | CB  | ASP | A | 55 | -5.494  | 39.232 | 60.075 | 1.00 | 30.92  |
| ATOM | 417 | CG  | ASP | A | 55 | -5.397  | 38.103 | 61.037 | 1.00 | 35.96  |
| ATOM | 418 | OD1 | ASP | A | 55 | -6.049  | 38.07  |        |      |        |



|      |     |     |     |   |    |         |        |        |      |        |
|------|-----|-----|-----|---|----|---------|--------|--------|------|--------|
| ATOM | 436 | N   | ASP | A | 58 | -7.617  | 48.188 | 62.065 | 1.00 | 32.68  |
| ATOM | 437 | CA  | ASP | A | 58 | -7.895  | 49.545 | 61.665 | 1.00 | 35.27  |
| ATOM | 438 | C   | ASP | A | 58 | -7.894  | 49.710 | 60.149 | 1.00 | 38.24  |
| ATOM | 439 | O   | ASP | A | 58 | -7.289  | 50.627 | 59.571 | 1.00 | 35.86  |
| ATOM | 440 | CB  | ASP | A | 58 | -6.968  | 50.550 | 62.386 | 1.00 | 37.22  |
| ATOM | 441 | CG  | ASP | A | 58 | -7.041  | 50.393 | 63.880 | 1.00 | 50.71  |
| ATOM | 442 | OD1 | ASP | A | 58 | -8.073  | 50.136 | 64.478 | 1.00 | 57.20  |
| ATOM | 443 | OD2 | ASP | A | 58 | -5.878  | 50.562 | 64.463 | 1.00 | 45.82  |
| ATOM | 444 | N   | LEU | A | 59 | -8.604  | 48.796 | 59.516 | 1.00 | 37.68  |
| ATOM | 445 | CA  | LEU | A | 59 | -8.720  | 48.813 | 58.079 | 1.00 | 39.36  |
| ATOM | 446 | C   | LEU | A | 59 | -10.077 | 49.243 | 57.555 | 1.00 | 45.55  |
| ATOM | 447 | O   | LEU | A | 59 | -11.146 | 48.946 | 58.120 | 1.00 | 44.18  |
| ATOM | 448 | CB  | LEU | A | 59 | -8.265  | 47.506 | 57.422 | 1.00 | 38.42  |
| ATOM | 449 | CG  | LEU | A | 59 | -6.762  | 47.475 | 57.218 | 1.00 | 37.40  |
| ATOM | 450 | CD1 | LEU | A | 59 | -6.392  | 46.173 | 56.526 | 1.00 | 36.39  |
| ATOM | 451 | CD2 | LEU | A | 59 | -6.321  | 48.655 | 56.361 | 1.00 | 36.57  |
| ATOM | 452 | N   | THR | A | 60 | -9.984  | 49.949 | 56.437 | 1.00 | 42.59  |
| ATOM | 453 | CA  | THR | A | 60 | -11.132 | 50.483 | 55.734 | 1.00 | 42.63  |
| ATOM | 454 | C   | THR | A | 60 | -11.357 | 49.705 | 54.463 | 1.00 | 38.18  |
| ATOM | 455 | O   | THR | A | 60 | -10.632 | 49.856 | 53.454 | 1.00 | 34.33  |
| ATOM | 456 | CB  | THR | A | 60 | -11.030 | 52.028 | 55.532 | 1.00 | 65.15  |
| ATOM | 457 | OG1 | THR | A | 60 | -11.806 | 52.736 | 56.504 | 1.00 | 67.56  |
| ATOM | 458 | CG2 | THR | A | 60 | -11.345 | 52.480 | 54.104 | 1.00 | 56.89  |
| ATOM | 459 | N   | ILE | A | 61 | -12.360 | 48.847 | 54.571 | 1.00 | 33.39  |
| ATOM | 460 | CA  | ILE | A | 61 | -12.753 | 47.975 | 53.482 | 1.00 | 35.89  |
| ATOM | 461 | C   | ILE | A | 61 | -13.726 | 48.634 | 52.533 | 1.00 | 41.05  |
| ATOM | 462 | O   | ILE | A | 61 | -14.913 | 48.706 | 52.840 | 1.00 | 40.08  |
| ATOM | 463 | CB  | ILE | A | 61 | -13.403 | 46.670 | 53.944 | 1.00 | 39.71  |
| ATOM | 464 | CG1 | ILE | A | 61 | -12.482 | 45.826 | 54.832 | 1.00 | 39.90  |
| ATOM | 465 | CG2 | ILE | A | 61 | -13.788 | 45.900 | 52.691 | 1.00 | 38.96  |
| ATOM | 466 | CD1 | ILE | A | 61 | -11.027 | 45.851 | 54.358 | 1.00 | 49.61  |
| ATOM | 467 | N   | GLU | A | 62 | -13.219 | 49.080 | 51.391 | 1.00 | 40.23  |
| ATOM | 468 | CA  | GLU | A | 62 | -14.040 | 49.700 | 50.365 | 1.00 | 41.73  |
| ATOM | 469 | C   | GLU | A | 62 | -14.986 | 48.633 | 49.826 | 1.00 | 47.09  |
| ATOM | 470 | O   | GLU | A | 62 | -16.207 | 48.726 | 49.926 | 1.00 | 47.52  |
| ATOM | 471 | CB  | GLU | A | 62 | -13.138 | 50.272 | 49.239 | 1.00 | 44.08  |
| ATOM | 472 | CG  | GLU | A | 62 | -13.765 | 51.406 | 48.381 | 1.00 | 64.08  |
| ATOM | 473 | CD  | GLU | A | 62 | -14.686 | 50.946 | 47.256 | 1.00 | 100.00 |
| ATOM | 474 | OE1 | GLU | A | 62 | -15.458 | 50.002 | 47.376 | 1.00 | 100.00 |
| ATOM | 475 | OE2 | GLU | A | 62 | -14.591 | 51.670 | 46.146 | 1.00 | 75.11  |
| ATOM | 476 | N   | LYS | A | 63 | -14.399 | 47.580 | 49.267 | 1.00 | 43.46  |
| ATOM | 477 | CA  | LYS | A | 63 | -15.168 | 46.474 | 48.746 | 1.00 | 40.53  |
| ATOM | 478 | C   | LYS | A | 63 | -14.250 | 45.307 | 48.489 | 1.00 | 45.38  |
| ATOM | 479 | O   | LYS | A | 63 | -13.046 |        |        |      |        |



|      |     |     |     |   |    |         |        |        |      |        |
|------|-----|-----|-----|---|----|---------|--------|--------|------|--------|
| ATOM | 497 | CG1 | VAL | A | 65 | -14.520 | 42.037 | 42.189 | 1.00 | 42.79  |
| ATOM | 498 | CG2 | VAL | A | 65 | -14.264 | 43.874 | 43.883 | 1.00 | 45.05  |
| ATOM | 499 | N   | ILE | A | 66 | -14.515 | 39.402 | 43.556 | 1.00 | 38.68  |
| ATOM | 500 | CA  | ILE | A | 66 | -14.179 | 38.053 | 43.113 | 1.00 | 39.98  |
| ATOM | 501 | C   | ILE | A | 66 | -14.899 | 37.774 | 41.802 | 1.00 | 44.86  |
| ATOM | 502 | O   | ILE | A | 66 | -16.136 | 37.735 | 41.729 | 1.00 | 42.69  |
| ATOM | 503 | CB  | ILE | A | 66 | -14.520 | 36.947 | 44.113 | 1.00 | 44.28  |
| ATOM | 504 | CG1 | ILE | A | 66 | -13.813 | 37.127 | 45.445 | 1.00 | 47.27  |
| ATOM | 505 | CG2 | ILE | A | 66 | -14.141 | 35.578 | 43.550 | 1.00 | 42.84  |
| ATOM | 506 | CD1 | ILE | A | 66 | -14.352 | 36.169 | 46.514 | 1.00 | 38.79  |
| ATOM | 507 | N   | ASN | A | 67 | -14.120 | 37.549 | 40.759 | 1.00 | 42.94  |
| ATOM | 508 | CA  | ASN | A | 67 | -14.715 | 37.266 | 39.472 | 1.00 | 44.24  |
| ATOM | 509 | C   | ASN | A | 67 | -15.541 | 38.444 | 39.008 | 1.00 | 54.25  |
| ATOM | 510 | O   | ASN | A | 67 | -16.743 | 38.344 | 38.768 | 1.00 | 57.56  |
| ATOM | 511 | CB  | ASN | A | 67 | -15.595 | 36.007 | 39.507 | 1.00 | 40.72  |
| ATOM | 512 | CG  | ASN | A | 67 | -14.788 | 34.759 | 39.745 | 1.00 | 57.39  |
| ATOM | 513 | OD1 | ASN | A | 67 | -13.581 | 34.711 | 39.454 | 1.00 | 52.63  |
| ATOM | 514 | ND2 | ASN | A | 67 | -15.446 | 33.760 | 40.317 | 1.00 | 44.54  |
| ATOM | 515 | N   | GLY | A | 68 | -14.876 | 39.574 | 38.899 | 1.00 | 50.43  |
| ATOM | 516 | CA  | GLY | A | 68 | -15.517 | 40.796 | 38.462 | 1.00 | 48.89  |
| ATOM | 517 | C   | GLY | A | 68 | -16.807 | 41.115 | 39.194 | 1.00 | 48.77  |
| ATOM | 518 | O   | GLY | A | 68 | -17.523 | 42.018 | 38.803 | 1.00 | 51.39  |
| ATOM | 519 | N   | GLN | A | 69 | -17.129 | 40.385 | 40.244 | 1.00 | 40.06  |
| ATOM | 520 | CA  | GLN | A | 69 | -18.348 | 40.716 | 40.928 | 1.00 | 40.02  |
| ATOM | 521 | C   | GLN | A | 69 | -18.031 | 41.059 | 42.364 | 1.00 | 50.45  |
| ATOM | 522 | O   | GLN | A | 69 | -16.943 | 40.748 | 42.855 | 1.00 | 50.53  |
| ATOM | 523 | CB  | GLN | A | 69 | -19.415 | 39.602 | 40.829 | 1.00 | 40.78  |
| ATOM | 524 | CG  | GLN | A | 69 | -19.966 | 39.367 | 39.414 | 1.00 | 23.77  |
| ATOM | 525 | CD  | GLN | A | 69 | -20.513 | 40.646 | 38.831 | 1.00 | 56.53  |
| ATOM | 526 | OE1 | GLN | A | 69 | -19.974 | 41.198 | 37.859 | 1.00 | 55.28  |
| ATOM | 527 | NE2 | GLN | A | 69 | -21.588 | 41.134 | 39.437 | 1.00 | 62.26  |
| ATOM | 528 | N   | GLU | A | 70 | -18.975 | 41.718 | 43.028 | 1.00 | 49.43  |
| ATOM | 529 | CA  | GLU | A | 70 | -18.766 | 42.094 | 44.407 | 1.00 | 50.67  |
| ATOM | 530 | C   | GLU | A | 70 | -19.296 | 40.996 | 45.288 | 1.00 | 57.90  |
| ATOM | 531 | O   | GLU | A | 70 | -20.272 | 40.367 | 44.909 | 1.00 | 63.90  |
| ATOM | 532 | CB  | GLU | A | 70 | -19.449 | 43.434 | 44.732 | 1.00 | 52.26  |
| ATOM | 533 | CG  | GLU | A | 70 | -18.824 | 44.624 | 43.970 | 1.00 | 64.80  |
| ATOM | 534 | CD  | GLU | A | 70 | -19.181 | 45.967 | 44.555 | 1.00 | 91.82  |
| ATOM | 535 | OE1 | GLU | A | 70 | -19.749 | 46.108 | 45.629 | 1.00 | 100.00 |
| ATOM | 536 | OE2 | GLU | A | 70 | -18.814 | 46.963 | 43.785 | 1.00 | 76.01  |
| ATOM | 537 | N   | VAL | A | 71 | -18.655 | 40.742 | 46.433 | 1.00 | 47.28  |
| ATOM | 538 | CA  | VAL | A | 71 | -19.119 | 39.685 | 47.335 | 1.00 | 43.84  |
| ATOM | 539 | C   | VAL | A | 71 | -19.434 | 40.153 | 48.768 | 1.00 | 41.62  |
| ATOM | 540 | O   | VAL | A | 71 | -18.983 | 41.206 | 49.254 | 1.00 | 35.70  |
| ATOM | 541 | CB  | VAL | A | 71 | -18.308 | 38.361 | 47.273 | 1.00 | 46.05  |
| ATOM | 542 | CG1 | VAL | A | 71 | -18.062 | 37.923 | 45.827 | 1.00 | 45.19  |
| ATOM | 543 | CG2 | VAL | A | 71 | -16.979 | 38.460 | 48.017 | 1.00 | 45.24  |
| ATOM | 544 | N   | LYS | A | 72 | -20.239 | 39.343 | 49.431 | 1.00 | 39.34  |
| ATOM | 545 | CA  | LYS | A | 72 | -20.610 | 39.594 | 50.792 | 1.00 | 42.40  |
| ATOM | 546 | C   | LYS | A | 72 | -19.347 | 39.466 | 51.668 | 1.00 | 56.92  |
| ATOM | 547 | O   | LYS | A | 72 | -18.399 | 38.729 | 51.334 | 1.00 | 59.27  |
| ATOM | 548 | CB  | LYS | A | 72 | -21.719 | 38.629 | 51.211 | 1.00 | 45.76  |
| ATOM | 549 | CG  | LYS | A | 72 | -22.378 | 38.960 | 52.557 | 1.00 | 86.98  |
| ATOM | 550 | CD  | LYS | A | 72 | -23.898 | 38.767 | 52.606 | 1.00 | 100.00 |
| ATOM | 551 | CE  | LYS | A | 72 | -24.656 | 40.012 | 53.077 | 1.00 | 100.00 |
| ATOM | 552 | NZ  | LYS | A | 72 | -26.011 | 39.730 | 53.592 | 1.00 | 100.00 |
| ATOM | 553 | N   | TYR | A | 73 | -19.332 | 40.210 | 52.780 | 1.00 | 55.45  |
| ATOM | 554 | CA  | TYR | A | 73 | -18.236 | 40.226 | 53.747 | 1.00 | 53.31  |
| ATOM | 555 | C   | TYR | A | 73 | -18.636 | 40.884 | 55.068 | 1.00 | 50.87  |
| ATOM | 556 | O   | TYR | A | 73 | -19.552 | 41.703 | 55.139 | 1.00 | 47.82  |
| ATOM | 557 | CB  | TYR | A | 73 | -16.891 | 40.741 | 53.214 | 1.00 | 52.73  |



|      |     |     |     |   |    |         |        |        |      |        |
|------|-----|-----|-----|---|----|---------|--------|--------|------|--------|
| ATOM | 558 | CG  | TYR | A | 73 | -16.765 | 42.244 | 53.227 | 1.00 | 51.76  |
| ATOM | 559 | CD1 | TYR | A | 73 | -16.539 | 42.946 | 54.416 | 1.00 | 52.82  |
| ATOM | 560 | CD2 | TYR | A | 73 | -16.927 | 42.967 | 52.039 | 1.00 | 53.30  |
| ATOM | 561 | CE1 | TYR | A | 73 | -16.439 | 44.340 | 54.422 | 1.00 | 52.71  |
| ATOM | 562 | CE2 | TYR | A | 73 | -16.804 | 44.359 | 52.026 | 1.00 | 55.39  |
| ATOM | 563 | CZ  | TYR | A | 73 | -16.592 | 45.044 | 53.229 | 1.00 | 63.45  |
| ATOM | 564 | OH  | TYR | A | 73 | -16.471 | 46.404 | 53.215 | 1.00 | 69.53  |
| ATOM | 565 | N   | ALA | A | 74 | -17.927 | 40.494 | 56.112 | 1.00 | 45.37  |
| ATOM | 566 | CA  | ALA | A | 74 | -18.180 | 40.999 | 57.433 | 1.00 | 42.62  |
| ATOM | 567 | C   | ALA | A | 74 | -16.892 | 41.265 | 58.222 | 1.00 | 47.81  |
| ATOM | 568 | O   | ALA | A | 74 | -15.894 | 40.554 | 58.133 | 1.00 | 45.55  |
| ATOM | 569 | CB  | ALA | A | 74 | -19.111 | 40.035 | 58.170 | 1.00 | 40.75  |
| ATOM | 570 | N   | LEU | A | 75 | -16.930 | 42.323 | 59.005 | 1.00 | 49.02  |
| ATOM | 571 | CA  | LEU | A | 75 | -15.829 | 42.693 | 59.869 | 1.00 | 48.85  |
| ATOM | 572 | C   | LEU | A | 75 | -16.319 | 42.464 | 61.281 | 1.00 | 47.18  |
| ATOM | 573 | O   | LEU | A | 75 | -17.309 | 43.021 | 61.687 | 1.00 | 44.35  |
| ATOM | 574 | CB  | LEU | A | 75 | -15.332 | 44.136 | 59.675 | 1.00 | 49.64  |
| ATOM | 575 | CG  | LEU | A | 75 | -14.789 | 44.357 | 58.270 | 1.00 | 58.09  |
| ATOM | 576 | CD1 | LEU | A | 75 | -14.524 | 45.841 | 58.023 | 1.00 | 61.34  |
| ATOM | 577 | CD2 | LEU | A | 75 | -13.512 | 43.565 | 58.069 | 1.00 | 62.34  |
| ATOM | 578 | N   | GLY | A | 76 | -15.647 | 41.592 | 62.004 | 1.00 | 47.67  |
| ATOM | 579 | CA  | GLY | A | 76 | -16.034 | 41.281 | 63.359 | 1.00 | 46.79  |
| ATOM | 580 | C   | GLY | A | 76 | -15.495 | 42.337 | 64.279 | 1.00 | 47.74  |
| ATOM | 581 | O   | GLY | A | 76 | -14.656 | 43.171 | 63.882 | 1.00 | 42.87  |
| ATOM | 582 | N   | GLU | A | 77 | -15.988 | 42.311 | 65.502 | 1.00 | 48.32  |
| ATOM | 583 | CA  | GLU | A | 77 | -15.526 | 43.300 | 66.431 | 1.00 | 52.14  |
| ATOM | 584 | C   | GLU | A | 77 | -14.029 | 43.195 | 66.679 | 1.00 | 56.71  |
| ATOM | 585 | O   | GLU | A | 77 | -13.418 | 42.120 | 66.591 | 1.00 | 55.78  |
| ATOM | 586 | CB  | GLU | A | 77 | -16.357 | 43.341 | 67.732 | 1.00 | 55.55  |
| ATOM | 587 | CG  | GLU | A | 77 | -17.198 | 42.063 | 67.969 | 1.00 | 79.57  |
| ATOM | 588 | CD  | GLU | A | 77 | -17.440 | 41.739 | 69.427 | 1.00 | 100.00 |
| ATOM | 589 | OE1 | GLU | A | 77 | -16.537 | 41.435 | 70.211 | 1.00 | 100.00 |
| ATOM | 590 | OE2 | GLU | A | 77 | -18.712 | 41.799 | 69.770 | 1.00 | 100.00 |
| ATOM | 591 | N   | ARG | A | 78 | -13.452 | 44.344 | 67.000 | 1.00 | 54.17  |
| ATOM | 592 | CA  | ARG | A | 78 | -12.041 | 44.433 | 67.298 | 1.00 | 53.38  |
| ATOM | 593 | C   | ARG | A | 78 | -11.627 | 43.656 | 68.579 | 1.00 | 58.88  |
| ATOM | 594 | O   | ARG | A | 78 | -12.247 | 43.767 | 69.635 | 1.00 | 61.35  |
| ATOM | 595 | CB  | ARG | A | 78 | -11.571 | 45.891 | 67.367 | 1.00 | 41.96  |
| ATOM | 596 | CG  | ARG | A | 78 | -10.050 | 46.006 | 67.326 | 1.00 | 38.20  |
| ATOM | 597 | CD  | ARG | A | 78 | -9.537  | 47.411 | 67.551 | 1.00 | 44.73  |
| ATOM | 598 | NE  | ARG | A | 78 | -8.294  | 47.648 | 66.842 | 1.00 | 66.47  |
| ATOM | 599 | CZ  | ARG | A | 78 | -7.250  | 48.247 | 67.389 | 1.00 | 97.61  |
| ATOM | 600 | NH1 | ARG | A | 78 | -7.276  | 48.692 | 68.645 | 1.00 | 100.00 |
| ATOM | 601 | NH2 | ARG |   |    |         |        |        |      |        |



00122110 022600

|      |     |     |     |   |    |         |        |        |      |       |
|------|-----|-----|-----|---|----|---------|--------|--------|------|-------|
| ATOM | 619 | C   | TYR | A | 81 | -4.163  | 43.116 | 68.285 | 1.00 | 30.82 |
| ATOM | 620 | O   | TYR | A | 81 | -3.480  | 43.215 | 67.269 | 1.00 | 34.48 |
| ATOM | 621 | CB  | TYR | A | 81 | -2.727  | 43.893 | 70.257 | 1.00 | 25.19 |
| ATOM | 622 | CG  | TYR | A | 81 | -2.713  | 42.491 | 70.839 | 1.00 | 24.57 |
| ATOM | 623 | CD1 | TYR | A | 81 | -3.327  | 42.247 | 72.066 | 1.00 | 27.27 |
| ATOM | 624 | CD2 | TYR | A | 81 | -2.165  | 41.410 | 70.148 | 1.00 | 21.82 |
| ATOM | 625 | CE1 | TYR | A | 81 | -3.380  | 40.975 | 72.632 | 1.00 | 26.49 |
| ATOM | 626 | CE2 | TYR | A | 81 | -2.230  | 40.122 | 70.682 | 1.00 | 23.48 |
| ATOM | 627 | CZ  | TYR | A | 81 | -2.827  | 39.908 | 71.930 | 1.00 | 38.28 |
| ATOM | 628 | OH  | TYR | A | 81 | -2.889  | 38.653 | 72.493 | 1.00 | 42.17 |
| ATOM | 629 | N   | LYS | A | 82 | -5.038  | 42.136 | 68.415 | 1.00 | 26.97 |
| ATOM | 630 | CA  | LYS | A | 82 | -5.170  | 41.229 | 67.293 | 1.00 | 27.99 |
| ATOM | 631 | C   | LYS | A | 82 | -5.867  | 41.898 | 66.072 | 1.00 | 38.90 |
| ATOM | 632 | O   | LYS | A | 82 | -5.614  | 41.541 | 64.900 | 1.00 | 37.15 |
| ATOM | 633 | CB  | LYS | A | 82 | -5.785  | 39.918 | 67.708 | 1.00 | 27.59 |
| ATOM | 634 | CG  | LYS | A | 82 | -5.169  | 39.451 | 69.008 | 1.00 | 39.68 |
| ATOM | 635 | CD  | LYS | A | 82 | -5.435  | 37.993 | 69.350 | 1.00 | 46.78 |
| ATOM | 636 | CE  | LYS | A | 82 | -6.414  | 37.819 | 70.492 | 1.00 | 59.84 |
| ATOM | 637 | NZ  | LYS | A | 82 | -7.097  | 36.523 | 70.452 | 1.00 | 63.48 |
| ATOM | 638 | N   | GLY | A | 83 | -6.738  | 42.894 | 66.367 | 1.00 | 35.64 |
| ATOM | 639 | CA  | GLY | A | 83 | -7.512  | 43.620 | 65.368 | 1.00 | 33.65 |
| ATOM | 640 | C   | GLY | A | 83 | -8.866  | 42.925 | 65.111 | 1.00 | 32.95 |
| ATOM | 641 | O   | GLY | A | 83 | -9.297  | 42.063 | 65.870 | 1.00 | 28.28 |
| ATOM | 642 | N   | SER | A | 84 | -9.535  | 43.300 | 64.026 | 1.00 | 34.51 |
| ATOM | 643 | CA  | SER | A | 84 | -10.839 | 42.742 | 63.673 | 1.00 | 36.13 |
| ATOM | 644 | C   | SER | A | 84 | -10.796 | 41.724 | 62.549 | 1.00 | 40.65 |
| ATOM | 645 | O   | SER | A | 84 | -10.173 | 41.893 | 61.501 | 1.00 | 39.77 |
| ATOM | 646 | CB  | SER | A | 84 | -11.883 | 43.808 | 63.383 | 1.00 | 37.68 |
| ATOM | 647 | OG  | SER | A | 84 | -11.812 | 44.832 | 64.352 | 1.00 | 45.14 |
| ATOM | 648 | N   | PRO | A | 85 | -11.491 | 40.656 | 62.791 | 1.00 | 37.01 |
| ATOM | 649 | CA  | PRO | A | 85 | -11.573 | 39.559 | 61.863 | 1.00 | 34.91 |
| ATOM | 650 | C   | PRO | A | 85 | -12.459 | 39.946 | 60.712 | 1.00 | 35.92 |
| ATOM | 651 | O   | PRO | A | 85 | -13.514 | 40.522 | 60.941 | 1.00 | 35.30 |
| ATOM | 652 | CB  | PRO | A | 85 | -12.227 | 38.406 | 62.647 | 1.00 | 37.00 |
| ATOM | 653 | CG  | PRO | A | 85 | -12.714 | 38.981 | 63.974 | 1.00 | 44.97 |
| ATOM | 654 | CD  | PRO | A | 85 | -12.325 | 40.462 | 64.004 | 1.00 | 40.72 |
| ATOM | 655 | N   | MET | A | 86 | -12.018 | 39.642 | 59.487 | 1.00 | 30.47 |
| ATOM | 656 | CA  | MET | A | 86 | -12.756 | 39.960 | 58.275 | 1.00 | 28.55 |
| ATOM | 657 | C   | MET | A | 86 | -13.165 | 38.683 | 57.552 | 1.00 | 40.49 |
| ATOM | 658 | O   | MET | A | 86 | -12.338 | 38.015 | 56.954 | 1.00 | 39.69 |
| ATOM | 659 | CB  | MET | A | 86 | -11.921 | 40.829 | 57.337 | 1.00 | 29.51 |
| ATOM | 660 | CG  | MET | A | 86 | -12.750 | 41.242 | 56.136 | 1.00 | 37.40 |
| ATOM | 661 | SD  | MET | A | 86 | -11.816 | 41.878 | 54.701 | 1.00 | 47.84 |
| ATOM | 662 | CE  | MET | A | 86 | -13.244 | 42.527 | 53.805 | 1.00 | 46.52 |
| ATOM | 663 | N   | GLU | A | 87 | -14.441 | 38.324 | 57.610 | 1.00 | 44.34 |
| ATOM | 664 | CA  | GLU | A | 87 | -14.912 | 37.107 | 56.950 | 1.00 | 47.21 |
| ATOM | 665 | C   | GLU | A | 87 | -15.495 | 37.352 | 55.560 | 1.00 | 51.53 |
| ATOM | 666 | O   | GLU | A | 87 | -16.425 | 38.129 | 55.424 | 1.00 | 53.92 |
| ATOM | 667 | CB  | GLU | A | 87 | -15.942 | 36.390 | 57.813 | 1.00 | 49.46 |
| ATOM | 668 | CG  | GLU | A | 87 | -16.144 | 34.937 | 57.389 | 1.00 | 56.39 |
| ATOM | 669 | CD  | GLU | A | 87 | -17.300 | 34.316 | 58.104 | 1.00 | 80.78 |
| ATOM | 670 | OE1 | GLU | A | 87 | -18.439 | 34.738 | 57.994 | 1.00 | 86.69 |
| ATOM | 671 | OE2 | GLU | A | 87 | -16.943 | 33.301 | 58.868 | 1.00 | 68.69 |
| ATOM | 672 | N   | ILE | A | 88 | -14.942 | 36.659 | 54.544 | 1.00 | 43.84 |
| ATOM | 673 | CA  | ILE | A | 88 | -15.332 | 36.765 | 53.145 | 1.00 | 40.15 |
| ATOM | 674 | C   | ILE | A | 88 | -16.145 | 35.610 | 52.613 | 1.00 | 46.72 |
| ATOM | 675 | O   | ILE | A | 88 | -15.725 | 34.460 | 52.656 | 1.00 | 48.10 |
| ATOM | 676 | CB  | ILE | A | 88 | -14.107 | 36.891 | 52.292 | 1.00 | 39.13 |
| ATOM | 677 | CG1 | ILE | A | 88 | -13.328 | 38.146 | 52.696 | 1.00 | 38.40 |
| ATOM | 678 | CG2 | ILE | A | 88 | -14.538 | 36.932 | 50.839 | 1.00 | 28.13 |
| ATOM | 679 | CD1 | ILE | A | 88 | -11.944 | 38.200 | 52.051 | 1.00 | 30.07 |



|      |     |     |     |   |    |         |        |        |      |        |
|------|-----|-----|-----|---|----|---------|--------|--------|------|--------|
| ATOM | 680 | N   | SER | A | 89 | -17.314 | 35.931 | 52.077 | 1.00 | 45.16  |
| ATOM | 681 | CA  | SER | A | 89 | -18.181 | 34.893 | 51.559 | 1.00 | 44.76  |
| ATOM | 682 | C   | SER | A | 89 | -17.902 | 34.531 | 50.131 | 1.00 | 46.01  |
| ATOM | 683 | O   | SER | A | 89 | -18.048 | 35.347 | 49.243 | 1.00 | 44.34  |
| ATOM | 684 | CB  | SER | A | 89 | -19.657 | 35.121 | 51.827 | 1.00 | 51.87  |
| ATOM | 685 | OG  | SER | A | 89 | -19.942 | 34.834 | 53.198 | 1.00 | 69.07  |
| ATOM | 686 | N   | LEU | A | 90 | -17.494 | 33.279 | 49.914 | 1.00 | 46.43  |
| ATOM | 687 | CA  | LEU | A | 90 | -17.204 | 32.804 | 48.575 | 1.00 | 46.93  |
| ATOM | 688 | C   | LEU | A | 90 | -18.450 | 32.235 | 47.935 | 1.00 | 55.26  |
| ATOM | 689 | O   | LEU | A | 90 | -19.210 | 31.476 | 48.556 | 1.00 | 54.94  |
| ATOM | 690 | CB  | LEU | A | 90 | -16.080 | 31.750 | 48.521 | 1.00 | 46.14  |
| ATOM | 691 | CG  | LEU | A | 90 | -15.262 | 31.607 | 49.792 | 1.00 | 50.78  |
| ATOM | 692 | CD1 | LEU | A | 90 | -14.546 | 30.261 | 49.806 | 1.00 | 50.27  |
| ATOM | 693 | CD2 | LEU | A | 90 | -14.219 | 32.708 | 49.863 | 1.00 | 55.52  |
| ATOM | 694 | N   | PRO | A | 91 | -18.626 | 32.607 | 46.683 | 1.00 | 54.81  |
| ATOM | 695 | CA  | PRO | A | 91 | -19.756 | 32.183 | 45.870 | 1.00 | 58.45  |
| ATOM | 696 | C   | PRO | A | 91 | -19.585 | 30.782 | 45.254 | 1.00 | 67.78  |
| ATOM | 697 | O   | PRO | A | 91 | -20.500 | 30.250 | 44.623 | 1.00 | 68.64  |
| ATOM | 698 | CB  | PRO | A | 91 | -19.843 | 33.213 | 44.738 | 1.00 | 59.70  |
| ATOM | 699 | CG  | PRO | A | 91 | -18.503 | 33.952 | 44.711 | 1.00 | 61.25  |
| ATOM | 700 | CD  | PRO | A | 91 | -17.731 | 33.539 | 45.961 | 1.00 | 54.16  |
| ATOM | 701 | N   | ILE | A | 92 | -18.413 | 30.177 | 45.416 | 1.00 | 64.82  |
| ATOM | 702 | CA  | ILE | A | 92 | -18.210 | 28.863 | 44.850 | 1.00 | 65.03  |
| ATOM | 703 | C   | ILE | A | 92 | -17.485 | 27.948 | 45.801 | 1.00 | 66.34  |
| ATOM | 704 | O   | ILE | A | 92 | -16.258 | 27.984 | 45.865 | 1.00 | 70.20  |
| ATOM | 705 | CB  | ILE | A | 92 | -17.433 | 28.927 | 43.547 | 1.00 | 69.56  |
| ATOM | 706 | CG1 | ILE | A | 92 | -18.298 | 29.495 | 42.430 | 1.00 | 70.02  |
| ATOM | 707 | CG2 | ILE | A | 92 | -16.975 | 27.517 | 43.171 | 1.00 | 71.86  |
| ATOM | 708 | CD1 | ILE | A | 92 | -17.528 | 29.672 | 41.121 | 1.00 | 80.63  |
| ATOM | 709 | N   | ALA | A | 93 | -18.219 | 27.115 | 46.534 | 1.00 | 54.40  |
| ATOM | 710 | CA  | ALA | A | 93 | -17.526 | 26.247 | 47.452 | 1.00 | 51.74  |
| ATOM | 711 | C   | ALA | A | 93 | -16.265 | 25.750 | 46.804 | 1.00 | 52.66  |
| ATOM | 712 | O   | ALA | A | 93 | -16.288 | 25.319 | 45.662 | 1.00 | 49.87  |
| ATOM | 713 | CB  | ALA | A | 93 | -18.367 | 25.101 | 47.968 | 1.00 | 52.76  |
| ATOM | 714 | N   | LEU | A | 94 | -15.162 | 25.861 | 47.544 | 1.00 | 48.18  |
| ATOM | 715 | CA  | LEU | A | 94 | -13.862 | 25.425 | 47.067 | 1.00 | 43.27  |
| ATOM | 716 | C   | LEU | A | 94 | -13.566 | 24.066 | 47.581 | 1.00 | 43.98  |
| ATOM | 717 | O   | LEU | A | 94 | -14.086 | 23.633 | 48.601 | 1.00 | 44.63  |
| ATOM | 718 | CB  | LEU | A | 94 | -12.713 | 26.344 | 47.509 | 1.00 | 41.05  |
| ATOM | 719 | CG  | LEU | A | 94 | -12.685 | 27.638 | 46.739 | 1.00 | 40.03  |
| ATOM | 720 | CD1 | LEU | A | 94 | -11.272 | 28.200 | 46.751 | 1.00 | 36.88  |
| ATOM | 721 | CD2 | LEU | A | 94 | -13.115 | 27.343 | 45.311 | 1.00 | 44.98  |
| ATOM | 722 | N   | SER | A | 95 | -12.706 | 23.406 | 46.875 | 1.00 | 43.26  |
| ATOM | 723 | CA  | SER | A | 95 | -12.321 | 22.074 | 47.256 | 1.00 | 43.76  |
| ATOM | 724 | C   | SER | A | 95 | -10.807 | 21.991 | 47.344 | 1.00 | 38.58  |
| ATOM | 725 | O   | SER | A | 95 | -10.087 | 22.944 | 46.975 | 1.00 | 36.78  |
| ATOM | 726 | CB  | SER | A | 95 | -12.902 | 21.092 | 46.256 | 1.00 | 51.55  |
| ATOM | 727 | OG  | SER | A | 95 | -14.299 | 21.305 | 46.156 | 1.00 | 62.74  |
| ATOM | 728 | N   | LYS | A | 96 | -10.321 | 20.863 | 47.830 | 1.00 | 31.10  |
| ATOM | 729 | CA  | LYS | A | 96 | -8.883  | 20.723 | 47.958 | 1.00 | 34.92  |
| ATOM | 730 | C   | LYS | A | 96 | -8.058  | 21.238 | 46.777 | 1.00 | 45.63  |
| ATOM | 731 | O   | LYS | A | 96 | -8.400  | 21.063 | 45.612 | 1.00 | 49.35  |
| ATOM | 732 | CB  | LYS | A | 96 | -8.401  | 19.366 | 48.451 | 1.00 | 38.53  |
| ATOM | 733 | CG  | LYS | A | 96 | -9.189  | 18.871 | 49.651 | 1.00 | 68.97  |
| ATOM | 734 | CD  | LYS | A | 96 | -8.691  | 17.549 | 50.221 | 1.00 | 80.86  |
| ATOM | 735 | CE  | LYS | A | 96 | -9.596  | 17.011 | 51.330 | 1.00 | 92.53  |
| ATOM | 736 | NZ  | LYS | A | 96 | -9.049  | 15.833 | 52.029 | 1.00 | 100.00 |
| ATOM | 737 | N   | ASN | A | 97 | -6.944  | 21.873 | 47.108 | 1.00 | 41.92  |
| ATOM | 738 | CA  | ASN | A | 97 | -6.009  | 22.403 | 46.139 | 1.00 | 40.91  |
| ATOM | 739 | C   | ASN | A | 97 | -6.606  | 23.348 | 45.088 | 1.00 | 42.64  |
| ATOM | 740 | O   | ASN | A | 97 | -5.963  | 23.681 | 44.068 | 1.00 | 38.69  |



00123410 022600

|      |     |     |     |   |     |         |        |        |      |       |
|------|-----|-----|-----|---|-----|---------|--------|--------|------|-------|
| ATOM | 741 | CB  | ASN | A | 97  | -5.084  | 21.304 | 45.583 | 1.00 | 28.16 |
| ATOM | 742 | CG  | ASN | A | 97  | -4.327  | 20.568 | 46.677 | 1.00 | 52.21 |
| ATOM | 743 | OD1 | ASN | A | 97  | -3.089  | 20.627 | 46.744 | 1.00 | 55.30 |
| ATOM | 744 | ND2 | ASN | A | 97  | -5.060  | 19.858 | 47.533 | 1.00 | 53.87 |
| ATOM | 745 | N   | GLN | A | 98  | -7.833  | 23.791 | 45.382 | 1.00 | 36.59 |
| ATOM | 746 | CA  | GLN | A | 98  | -8.557  | 24.718 | 44.536 | 1.00 | 38.44 |
| ATOM | 747 | C   | GLN | A | 98  | -8.288  | 26.181 | 44.951 | 1.00 | 43.30 |
| ATOM | 748 | O   | GLN | A | 98  | -8.248  | 26.526 | 46.138 | 1.00 | 43.40 |
| ATOM | 749 | CB  | GLN | A | 98  | -10.064 | 24.395 | 44.575 | 1.00 | 42.26 |
| ATOM | 750 | CG  | GLN | A | 98  | -10.553 | 23.538 | 43.385 | 1.00 | 68.24 |
| ATOM | 751 | CD  | GLN | A | 98  | -12.008 | 23.778 | 43.010 | 1.00 | 95.57 |
| ATOM | 752 | OE1 | GLN | A | 98  | -12.890 | 22.935 | 43.278 | 1.00 | 86.92 |
| ATOM | 753 | NE2 | GLN | A | 98  | -12.271 | 24.935 | 42.393 | 1.00 | 95.48 |
| ATOM | 754 | N   | GLU | A | 99  | -8.089  | 27.062 | 43.973 | 1.00 | 39.70 |
| ATOM | 755 | CA  | GLU | A | 99  | -7.817  | 28.468 | 44.280 | 1.00 | 40.49 |
| ATOM | 756 | C   | GLU | A | 99  | -8.750  | 29.536 | 43.683 | 1.00 | 47.84 |
| ATOM | 757 | O   | GLU | A | 99  | -9.330  | 29.394 | 42.606 | 1.00 | 46.85 |
| ATOM | 758 | CB  | GLU | A | 99  | -6.361  | 28.866 | 43.951 | 1.00 | 40.24 |
| ATOM | 759 | CG  | GLU | A | 99  | -5.608  | 27.861 | 43.080 | 1.00 | 44.16 |
| ATOM | 760 | CD  | GLU | A | 99  | -4.120  | 28.119 | 42.990 | 1.00 | 65.64 |
| ATOM | 761 | OE1 | GLU | A | 99  | -3.636  | 29.062 | 42.376 | 1.00 | 73.95 |
| ATOM | 762 | OE2 | GLU | A | 99  | -3.395  | 27.210 | 43.614 | 1.00 | 55.99 |
| ATOM | 763 | N   | ILE | A | 100 | -8.848  | 30.643 | 44.418 | 1.00 | 43.55 |
| ATOM | 764 | CA  | ILE | A | 100 | -9.595  | 31.800 | 44.005 | 1.00 | 43.46 |
| ATOM | 765 | C   | ILE | A | 100 | -8.701  | 32.992 | 44.238 | 1.00 | 53.31 |
| ATOM | 766 | O   | ILE | A | 100 | -7.725  | 32.927 | 45.004 | 1.00 | 55.16 |
| ATOM | 767 | CB  | ILE | A | 100 | -10.881 | 32.068 | 44.773 | 1.00 | 46.65 |
| ATOM | 768 | CG1 | ILE | A | 100 | -10.762 | 31.640 | 46.227 | 1.00 | 50.76 |
| ATOM | 769 | CG2 | ILE | A | 100 | -12.111 | 31.486 | 44.106 | 1.00 | 46.76 |
| ATOM | 770 | CD1 | ILE | A | 100 | -9.959  | 32.620 | 47.087 | 1.00 | 64.36 |
| ATOM | 771 | N   | VAL | A | 101 | -9.060  | 34.076 | 43.580 | 1.00 | 48.20 |
| ATOM | 772 | CA  | VAL | A | 101 | -8.382  | 35.329 | 43.760 | 1.00 | 45.63 |
| ATOM | 773 | C   | VAL | A | 101 | -9.383  | 36.351 | 44.295 | 1.00 | 48.59 |
| ATOM | 774 | O   | VAL | A | 101 | -10.331 | 36.722 | 43.623 | 1.00 | 51.29 |
| ATOM | 775 | CB  | VAL | A | 101 | -7.461  | 35.793 | 42.633 | 1.00 | 45.06 |
| ATOM | 776 | CG1 | VAL | A | 101 | -7.693  | 35.000 | 41.378 | 1.00 | 43.25 |
| ATOM | 777 | CG2 | VAL | A | 101 | -7.609  | 37.289 | 42.395 | 1.00 | 45.02 |
| ATOM | 778 | N   | ILE | A | 102 | -9.182  | 36.738 | 45.546 | 1.00 | 41.15 |
| ATOM | 779 | CA  | ILE | A | 102 | -10.023 | 37.690 | 46.238 | 1.00 | 39.43 |
| ATOM | 780 | C   | ILE | A | 102 | -9.439  | 39.062 | 46.170 | 1.00 | 49.35 |
| ATOM | 781 | O   | ILE | A | 102 | -8.331  | 39.274 | 46.659 | 1.00 | 53.80 |
| ATOM | 782 | CB  | ILE | A | 102 | -10.097 | 37.319 | 47.694 | 1.00 | 39.19 |
| ATOM | 783 | CG1 | ILE | A | 102 | -10.180 | 35.800 | 47.809 | 1.00 | 35.28 |
| ATOM | 784 | CG2 | ILE | A | 102 | -11.300 | 37.992 | 48.341 | 1.00 | 35.25 |
| ATOM | 785 | CD1 | ILE | A | 102 | -10.962 | 35.392 | 49.044 | 1.00 | 47.09 |
| ATOM | 786 | N   | GLU | A | 103 | -10.192 | 39.984 | 45.572 | 1.00 | 43.20 |
| ATOM | 787 | CA  | GLU | A | 103 | -9.748  | 41.362 | 45.433 | 1.00 | 39.88 |
| ATOM | 788 | C   | GLU | A | 103 | -10.378 | 42.299 | 46.425 | 1.00 | 44.03 |
| ATOM | 789 | O   | GLU | A | 103 | -11.580 | 42.558 | 46.385 | 1.00 | 41.34 |
| ATOM | 790 | CB  | GLU | A | 103 | -9.950  | 41.930 | 44.047 | 1.00 | 39.11 |
| ATOM | 791 | CG  | GLU | A | 103 | -9.017  | 43.112 | 43.863 | 1.00 | 36.18 |
| ATOM | 792 | CD  | GLU | A | 103 | -9.150  | 43.666 | 42.485 | 1.00 | 61.93 |
| ATOM | 793 | OE1 | GLU | A | 103 | -10.157 | 44.234 | 42.100 | 1.00 | 69.89 |
| ATOM | 794 | OE2 | GLU | A | 103 | -8.087  | 43.457 | 41.744 | 1.00 | 76.18 |
| ATOM | 795 | N   | ILE | A | 104 | -9.534  | 42.797 | 47.322 | 1.00 | 42.69 |
| ATOM | 796 | CA  | ILE | A | 104 | -9.969  | 43.718 | 48.346 | 1.00 | 40.72 |
| ATOM | 797 | C   | ILE | A | 104 | -9.522  | 45.167 | 48.099 | 1.00 | 46.21 |
| ATOM | 798 | O   | ILE | A | 104 | -8.346  | 45.478 | 47.866 | 1.00 | 42.68 |
| ATOM | 799 | CB  | ILE | A | 104 | -9.578  | 43.283 | 49.754 | 1.00 | 41.75 |
| ATOM | 800 | CG1 | ILE | A | 104 | -10.006 | 41.855 | 50.032 | 1.00 | 39.85 |
| ATOM | 801 | CG2 | ILE | A | 104 | -10.225 | 44.222 | 50.768 | 1.00 | 41.53 |



|      |     |     |     |   |     |         |        |        |      |        |
|------|-----|-----|-----|---|-----|---------|--------|--------|------|--------|
| ATOM | 802 | CD1 | ILE | A | 104 | -8.839  | 40.995 | 50.485 | 1.00 | 34.17  |
| ATOM | 803 | N   | SER | A | 105 | -10.506 | 46.056 | 48.173 | 1.00 | 47.94  |
| ATOM | 804 | CA  | SER | A | 105 | -10.278 | 47.481 | 48.046 | 1.00 | 48.05  |
| ATOM | 805 | C   | SER | A | 105 | -10.184 | 47.977 | 49.482 | 1.00 | 42.39  |
| ATOM | 806 | O   | SER | A | 105 | -11.134 | 47.879 | 50.263 | 1.00 | 39.69  |
| ATOM | 807 | CB  | SER | A | 105 | -11.399 | 48.180 | 47.290 | 1.00 | 53.77  |
| ATOM | 808 | OG  | SER | A | 105 | -11.399 | 47.789 | 45.930 | 1.00 | 60.69  |
| ATOM | 809 | N   | PHE | A | 106 | -9.020  | 48.445 | 49.857 | 1.00 | 35.07  |
| ATOM | 810 | CA  | PHE | A | 106 | -8.844  | 48.890 | 51.223 | 1.00 | 34.98  |
| ATOM | 811 | C   | PHE | A | 106 | -8.177  | 50.238 | 51.262 | 1.00 | 39.26  |
| ATOM | 812 | O   | PHE | A | 106 | -7.607  | 50.730 | 50.265 | 1.00 | 34.24  |
| ATOM | 813 | CB  | PHE | A | 106 | -8.015  | 47.864 | 52.060 | 1.00 | 36.05  |
| ATOM | 814 | CG  | PHE | A | 106 | -6.581  | 47.815 | 51.556 | 1.00 | 37.24  |
| ATOM | 815 | CD1 | PHE | A | 106 | -6.251  | 47.073 | 50.422 | 1.00 | 39.71  |
| ATOM | 816 | CD2 | PHE | A | 106 | -5.579  | 48.579 | 52.161 | 1.00 | 36.44  |
| ATOM | 817 | CE1 | PHE | A | 106 | -4.950  | 47.086 | 49.920 | 1.00 | 41.48  |
| ATOM | 818 | CE2 | PHE | A | 106 | -4.273  | 48.609 | 51.672 | 1.00 | 38.19  |
| ATOM | 819 | CZ  | PHE | A | 106 | -3.961  | 47.856 | 50.540 | 1.00 | 37.91  |
| ATOM | 820 | N   | GLU | A | 107 | -8.284  | 50.794 | 52.453 | 1.00 | 40.64  |
| ATOM | 821 | CA  | GLU | A | 107 | -7.711  | 52.064 | 52.848 | 1.00 | 43.81  |
| ATOM | 822 | C   | GLU | A | 107 | -7.206  | 51.869 | 54.284 | 1.00 | 43.82  |
| ATOM | 823 | O   | GLU | A | 107 | -7.933  | 51.303 | 55.121 | 1.00 | 38.38  |
| ATOM | 824 | CB  | GLU | A | 107 | -8.737  | 53.234 | 52.753 | 1.00 | 46.93  |
| ATOM | 825 | CG  | GLU | A | 107 | -8.107  | 54.637 | 52.467 | 1.00 | 67.21  |
| ATOM | 826 | CD  | GLU | A | 107 | -9.086  | 55.715 | 52.042 | 1.00 | 100.00 |
| ATOM | 827 | OE1 | GLU | A | 107 | -10.208 | 55.504 | 51.599 | 1.00 | 100.00 |
| ATOM | 828 | OE2 | GLU | A | 107 | -8.631  | 56.938 | 52.221 | 1.00 | 93.72  |
| ATOM | 829 | N   | THR | A | 108 | -5.963  | 52.294 | 54.551 | 1.00 | 39.12  |
| ATOM | 830 | CA  | THR | A | 108 | -5.345  | 52.175 | 55.873 | 1.00 | 39.69  |
| ATOM | 831 | C   | THR | A | 108 | -5.564  | 53.427 | 56.724 | 1.00 | 49.82  |
| ATOM | 832 | O   | THR | A | 108 | -5.565  | 54.552 | 56.177 | 1.00 | 50.94  |
| ATOM | 833 | CB  | THR | A | 108 | -3.810  | 52.095 | 55.722 | 1.00 | 40.40  |
| ATOM | 834 | OG1 | THR | A | 108 | -3.360  | 53.226 | 54.981 | 1.00 | 32.22  |
| ATOM | 835 | CG2 | THR | A | 108 | -3.371  | 50.802 | 55.042 | 1.00 | 46.43  |
| ATOM | 836 | N   | SER | A | 109 | -5.698  | 53.217 | 58.065 | 1.00 | 42.02  |
| ATOM | 837 | CA  | SER | A | 109 | -5.848  | 54.294 | 59.038 | 1.00 | 38.13  |
| ATOM | 838 | C   | SER | A | 109 | -4.555  | 55.101 | 59.082 | 1.00 | 38.47  |
| ATOM | 839 | O   | SER | A | 109 | -3.460  | 54.583 | 58.921 | 1.00 | 33.60  |
| ATOM | 840 | CB  | SER | A | 109 | -6.166  | 53.759 | 60.437 | 1.00 | 41.44  |
| ATOM | 841 | OG  | SER | A | 109 | -6.205  | 54.812 | 61.404 | 1.00 | 47.63  |
| ATOM | 842 | N   | PRO | A | 110 | -4.655  | 56.392 | 59.308 | 1.00 | 41.64  |
| ATOM | 843 | CA  | PRO | A | 110 | -3.419  | 57.116 | 59.393 | 1.00 | 40.75  |
| ATOM | 844 | C   | PRO | A | 110 | -2.803  | 56.749 | 60.725 | 1.00 | 41.47  |
| ATOM | 845 | O   | PRO | A | 110 | -       |        |        |      |        |



6012210-022222

|      |     |     |           |        |        |        |      |       |
|------|-----|-----|-----------|--------|--------|--------|------|-------|
| ATOM | 863 | OG  | SER A 112 | -0.682 | 50.814 | 59.762 | 1.00 | 31.94 |
| ATOM | 864 | N   | SER A 113 | -0.666 | 50.872 | 63.033 | 1.00 | 31.84 |
| ATOM | 865 | CA  | SER A 113 | 0.445  | 50.460 | 63.866 | 1.00 | 29.27 |
| ATOM | 866 | C   | SER A 113 | 1.601  | 49.927 | 63.040 | 1.00 | 33.37 |
| ATOM | 867 | O   | SER A 113 | 2.715  | 49.792 | 63.497 | 1.00 | 32.95 |
| ATOM | 868 | CB  | SER A 113 | 0.052  | 49.498 | 64.945 | 1.00 | 29.45 |
| ATOM | 869 | OG  | SER A 113 | 0.045  | 48.169 | 64.462 | 1.00 | 34.27 |
| ATOM | 870 | N   | ALA A 114 | 1.357  | 49.628 | 61.797 | 1.00 | 33.69 |
| ATOM | 871 | CA  | ALA A 114 | 2.437  | 49.134 | 60.981 | 1.00 | 34.05 |
| ATOM | 872 | C   | ALA A 114 | 3.239  | 50.287 | 60.388 | 1.00 | 37.83 |
| ATOM | 873 | O   | ALA A 114 | 4.411  | 50.149 | 60.033 | 1.00 | 37.72 |
| ATOM | 874 | CB  | ALA A 114 | 1.845  | 48.292 | 59.852 | 1.00 | 34.51 |
| ATOM | 875 | N   | LEU A 115 | 2.580  | 51.432 | 60.259 | 1.00 | 32.19 |
| ATOM | 876 | CA  | LEU A 115 | 3.201  | 52.595 | 59.662 | 1.00 | 30.48 |
| ATOM | 877 | C   | LEU A 115 | 3.509  | 53.745 | 60.565 | 1.00 | 35.32 |
| ATOM | 878 | O   | LEU A 115 | 2.902  | 54.012 | 61.604 | 1.00 | 35.25 |
| ATOM | 879 | CB  | LEU A 115 | 2.358  | 53.156 | 58.507 | 1.00 | 30.53 |
| ATOM | 880 | CG  | LEU A 115 | 1.787  | 52.064 | 57.602 | 1.00 | 35.51 |
| ATOM | 881 | CD1 | LEU A 115 | 0.812  | 52.710 | 56.637 | 1.00 | 35.12 |
| ATOM | 882 | CD2 | LEU A 115 | 2.903  | 51.387 | 56.821 | 1.00 | 33.88 |
| ATOM | 883 | N   | GLN A 116 | 4.490  | 54.457 | 60.096 | 1.00 | 34.00 |
| ATOM | 884 | CA  | GLN A 116 | 4.926  | 55.656 | 60.737 | 1.00 | 32.52 |
| ATOM | 885 | C   | GLN A 116 | 5.066  | 56.689 | 59.645 | 1.00 | 31.34 |
| ATOM | 886 | O   | GLN A 116 | 5.880  | 56.552 | 58.729 | 1.00 | 28.29 |
| ATOM | 887 | CB  | GLN A 116 | 6.232  | 55.540 | 61.496 | 1.00 | 32.66 |
| ATOM | 888 | CG  | GLN A 116 | 6.419  | 56.813 | 62.322 | 1.00 | 41.25 |
| ATOM | 889 | CD  | GLN A 116 | 7.777  | 56.897 | 62.952 | 1.00 | 50.08 |
| ATOM | 890 | OE1 | GLN A 116 | 8.515  | 55.905 | 63.017 | 1.00 | 55.36 |
| ATOM | 891 | NE2 | GLN A 116 | 8.090  | 58.081 | 63.438 | 1.00 | 38.23 |
| ATOM | 892 | N   | TRP A 117 | 4.210  | 57.680 | 59.748 | 1.00 | 26.66 |
| ATOM | 893 | CA  | TRP A 117 | 4.148  | 58.785 | 58.827 | 1.00 | 26.04 |
| ATOM | 894 | C   | TRP A 117 | 4.912  | 59.978 | 59.375 | 1.00 | 34.56 |
| ATOM | 895 | O   | TRP A 117 | 4.467  | 60.589 | 60.364 | 1.00 | 36.83 |
| ATOM | 896 | CB  | TRP A 117 | 2.669  | 59.188 | 58.630 | 1.00 | 23.15 |
| ATOM | 897 | CG  | TRP A 117 | 1.826  | 58.209 | 57.863 | 1.00 | 23.02 |
| ATOM | 898 | CD1 | TRP A 117 | 1.052  | 57.224 | 58.397 | 1.00 | 26.39 |
| ATOM | 899 | CD2 | TRP A 117 | 1.640  | 58.135 | 56.433 | 1.00 | 21.06 |
| ATOM | 900 | NE1 | TRP A 117 | 0.395  | 56.534 | 57.393 | 1.00 | 26.40 |
| ATOM | 901 | CE2 | TRP A 117 | 0.735  | 57.087 | 56.184 | 1.00 | 27.99 |
| ATOM | 902 | CE3 | TRP A 117 | 2.121  | 58.872 | 55.361 | 1.00 | 20.95 |
| ATOM | 903 | CZ2 | TRP A 117 | 0.352  | 56.753 | 54.886 | 1.00 | 28.21 |
| ATOM | 904 | CZ3 | TRP A 117 | 1.750  | 58.560 | 54.079 | 1.00 | 22.43 |
| ATOM | 905 | CH2 | TRP A 117 | 0.872  | 57.512 | 53.847 | 1.00 | 24.28 |
| ATOM | 906 | N   | LEU A 118 | 6.043  | 60.340 | 58.756 | 1.00 | 31.44 |
| ATOM | 907 | CA  | LEU A 118 | 6.745  | 61.506 | 59.276 | 1.00 | 36.67 |
| ATOM | 908 | C   | LEU A 118 | 6.584  | 62.774 | 58.432 | 1.00 | 46.93 |
| ATOM | 909 | O   | LEU A 118 | 6.434  | 62.705 | 57.210 | 1.00 | 51.17 |
| ATOM | 910 | CB  | LEU A 118 | 8.250  | 61.327 | 59.577 | 1.00 | 38.83 |
| ATOM | 911 | CG  | LEU A 118 | 8.881  | 59.939 | 59.398 | 1.00 | 44.33 |
| ATOM | 912 | CD1 | LEU A 118 | 10.392 | 60.065 | 59.569 | 1.00 | 42.12 |
| ATOM | 913 | CD2 | LEU A 118 | 8.351  | 58.950 | 60.426 | 1.00 | 49.99 |
| ATOM | 914 | N   | THR A 119 | 6.524  | 63.939 | 59.109 | 1.00 | 41.34 |
| ATOM | 915 | CA  | THR A 119 | 6.449  | 65.260 | 58.468 | 1.00 | 38.89 |
| ATOM | 916 | C   | THR A 119 | 7.847  | 65.633 | 58.034 | 1.00 | 40.14 |
| ATOM | 917 | O   | THR A 119 | 8.841  | 65.165 | 58.605 | 1.00 | 44.03 |
| ATOM | 918 | CB  | THR A 119 | 5.932  | 66.300 | 59.467 | 1.00 | 42.63 |
| ATOM | 919 | OG1 | THR A 119 | 6.994  | 66.605 | 60.362 | 1.00 | 50.01 |
| ATOM | 920 | CG2 | THR A 119 | 4.769  | 65.668 | 60.224 | 1.00 | 36.78 |
| ATOM | 921 | N   | PRO A 120 | 7.963  | 66.440 | 57.020 | 1.00 | 33.41 |
| ATOM | 922 | CA  | PRO A 120 | 9.275  | 66.781 | 56.517 | 1.00 | 33.18 |
| ATOM | 923 | C   | PRO A 120 | 10.260 | 67.209 | 57.599 | 1.00 | 38.27 |



|      |     |     |     |   |     |        |        |        |      |        |
|------|-----|-----|-----|---|-----|--------|--------|--------|------|--------|
| ATOM | 924 | O   | PRO | A | 120 | 11.433 | 66.829 | 57.566 | 1.00 | 34.42  |
| ATOM | 925 | CB  | PRO | A | 120 | 9.068  | 67.840 | 55.416 | 1.00 | 33.54  |
| ATOM | 926 | CG  | PRO | A | 120 | 7.582  | 67.823 | 55.097 | 1.00 | 34.86  |
| ATOM | 927 | CD  | PRO | A | 120 | 6.891  | 67.180 | 56.300 | 1.00 | 30.86  |
| ATOM | 928 | N   | GLU | A | 121 | 9.751  | 67.982 | 58.563 | 1.00 | 38.03  |
| ATOM | 929 | CA  | GLU | A | 121 | 10.534 | 68.474 | 59.681 | 1.00 | 41.03  |
| ATOM | 930 | C   | GLU | A | 121 | 11.212 | 67.361 | 60.411 | 1.00 | 50.88  |
| ATOM | 931 | O   | GLU | A | 121 | 12.279 | 67.548 | 60.977 | 1.00 | 54.97  |
| ATOM | 932 | CB  | GLU | A | 121 | 9.742  | 69.325 | 60.699 | 1.00 | 43.28  |
| ATOM | 933 | CG  | GLU | A | 121 | 8.220  | 69.071 | 60.702 | 1.00 | 64.72  |
| ATOM | 934 | CD  | GLU | A | 121 | 7.398  | 70.118 | 59.988 | 1.00 | 86.07  |
| ATOM | 935 | OE1 | GLU | A | 121 | 7.007  | 71.131 | 60.538 | 1.00 | 100.00 |
| ATOM | 936 | OE2 | GLU | A | 121 | 7.108  | 69.803 | 58.739 | 1.00 | 59.72  |
| ATOM | 937 | N   | GLN | A | 122 | 10.569 | 66.202 | 60.394 | 1.00 | 44.09  |
| ATOM | 938 | CA  | GLN | A | 122 | 11.083 | 65.019 | 61.041 | 1.00 | 40.20  |
| ATOM | 939 | C   | GLN | A | 122 | 12.170 | 64.373 | 60.232 | 1.00 | 47.73  |
| ATOM | 940 | O   | GLN | A | 122 | 12.711 | 63.343 | 60.643 | 1.00 | 53.29  |
| ATOM | 941 | CB  | GLN | A | 122 | 9.965  | 63.992 | 61.224 | 1.00 | 39.31  |
| ATOM | 942 | CG  | GLN | A | 122 | 9.057  | 64.441 | 62.361 | 1.00 | 30.23  |
| ATOM | 943 | CD  | GLN | A | 122 | 7.756  | 63.691 | 62.438 | 1.00 | 38.25  |
| ATOM | 944 | OE1 | GLN | A | 122 | 6.899  | 63.804 | 61.548 | 1.00 | 53.34  |
| ATOM | 945 | NE2 | GLN | A | 122 | 7.592  | 62.938 | 63.521 | 1.00 | 18.98  |
| ATOM | 946 | N   | THR | A | 123 | 12.486 | 64.942 | 59.074 | 1.00 | 38.99  |
| ATOM | 947 | CA  | THR | A | 123 | 13.490 | 64.319 | 58.229 | 1.00 | 36.00  |
| ATOM | 948 | C   | THR | A | 123 | 14.755 | 65.034 | 58.264 | 1.00 | 35.30  |
| ATOM | 949 | O   | THR | A | 123 | 14.842 | 66.074 | 58.875 | 1.00 | 34.95  |
| ATOM | 950 | CB  | THR | A | 123 | 13.067 | 64.145 | 56.759 | 1.00 | 38.25  |
| ATOM | 951 | OG1 | THR | A | 123 | 13.144 | 65.374 | 56.046 | 1.00 | 43.75  |
| ATOM | 952 | CG2 | THR | A | 123 | 11.643 | 63.616 | 56.725 | 1.00 | 40.72  |
| ATOM | 953 | N   | SER | A | 124 | 15.699 | 64.447 | 57.557 | 1.00 | 32.18  |
| ATOM | 954 | CA  | SER | A | 124 | 17.025 | 64.996 | 57.442 | 1.00 | 33.71  |
| ATOM | 955 | C   | SER | A | 124 | 17.007 | 66.216 | 56.553 | 1.00 | 39.04  |
| ATOM | 956 | O   | SER | A | 124 | 17.537 | 67.268 | 56.883 | 1.00 | 39.07  |
| ATOM | 957 | CB  | SER | A | 124 | 18.023 | 63.992 | 56.859 | 1.00 | 37.73  |
| ATOM | 958 | OG  | SER | A | 124 | 18.359 | 62.978 | 57.796 | 1.00 | 36.28  |
| ATOM | 959 | N   | GLY | A | 125 | 16.389 | 66.025 | 55.414 | 1.00 | 38.59  |
| ATOM | 960 | CA  | GLY | A | 125 | 16.280 | 67.034 | 54.396 | 1.00 | 39.90  |
| ATOM | 961 | C   | GLY | A | 125 | 15.290 | 68.094 | 54.749 | 1.00 | 46.83  |
| ATOM | 962 | O   | GLY | A | 125 | 15.347 | 69.171 | 54.172 | 1.00 | 49.78  |
| ATOM | 963 | N   | LYS | A | 126 | 14.391 | 67.788 | 55.678 | 1.00 | 41.09  |
| ATOM | 964 | CA  | LYS | A | 126 | 13.396 | 68.761 | 56.126 | 1.00 | 41.26  |
| ATOM | 965 | C   | LYS | A | 126 | 12.498 | 69.307 | 55.020 | 1.00 | 47.42  |
| ATOM | 966 | O   | LYS | A | 126 | 11.617 | 70.141 | 55.279 | 1.00 | 48.94  |
| ATOM |     |     |     |   |     |        |        |        |      |        |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 985  | CB  | HIS | A | 128 | 10.628 | 65.194 | 51.097 | 1.00 | 42.16 |
| ATOM | 986  | CG  | HIS | A | 128 | 10.947 | 65.936 | 49.854 | 1.00 | 47.24 |
| ATOM | 987  | ND1 | HIS | A | 128 | 9.943  | 66.423 | 49.029 | 1.00 | 49.12 |
| ATOM | 988  | CD2 | HIS | A | 128 | 12.159 | 66.262 | 49.322 | 1.00 | 51.13 |
| ATOM | 989  | CE1 | HIS | A | 128 | 10.559 | 67.031 | 48.026 | 1.00 | 49.97 |
| ATOM | 990  | NE2 | HIS | A | 128 | 11.888 | 66.953 | 48.166 | 1.00 | 50.87 |
| ATOM | 991  | N   | PRO | A | 129 | 8.447  | 64.572 | 53.171 | 1.00 | 32.55 |
| ATOM | 992  | CA  | PRO | A | 129 | 7.968  | 63.650 | 54.163 | 1.00 | 31.15 |
| ATOM | 993  | C   | PRO | A | 129 | 8.636  | 62.328 | 53.900 | 1.00 | 34.90 |
| ATOM | 994  | O   | PRO | A | 129 | 9.481  | 62.214 | 53.021 | 1.00 | 35.46 |
| ATOM | 995  | CB  | PRO | A | 129 | 6.466  | 63.490 | 53.986 | 1.00 | 31.94 |
| ATOM | 996  | CG  | PRO | A | 129 | 6.133  | 64.104 | 52.649 | 1.00 | 36.83 |
| ATOM | 997  | CD  | PRO | A | 129 | 7.384  | 64.850 | 52.185 | 1.00 | 32.71 |
| ATOM | 998  | N   | TYR | A | 130 | 8.248  | 61.342 | 54.659 | 1.00 | 29.47 |
| ATOM | 999  | CA  | TYR | A | 130 | 8.826  | 60.025 | 54.548 | 1.00 | 29.35 |
| ATOM | 1000 | C   | TYR | A | 130 | 7.856  | 59.046 | 55.156 | 1.00 | 31.83 |
| ATOM | 1001 | O   | TYR | A | 130 | 7.138  | 59.375 | 56.093 | 1.00 | 29.84 |
| ATOM | 1002 | CB  | TYR | A | 130 | 10.098 | 60.029 | 55.433 | 1.00 | 30.54 |
| ATOM | 1003 | CG  | TYR | A | 130 | 11.083 | 58.886 | 55.285 | 1.00 | 29.76 |
| ATOM | 1004 | CD1 | TYR | A | 130 | 10.845 | 57.630 | 55.845 | 1.00 | 26.16 |
| ATOM | 1005 | CD2 | TYR | A | 130 | 12.290 | 59.110 | 54.619 | 1.00 | 30.28 |
| ATOM | 1006 | CE1 | TYR | A | 130 | 11.795 | 56.621 | 55.721 | 1.00 | 17.87 |
| ATOM | 1007 | CE2 | TYR | A | 130 | 13.253 | 58.114 | 54.479 | 1.00 | 27.75 |
| ATOM | 1008 | CZ  | TYR | A | 130 | 12.983 | 56.866 | 55.031 | 1.00 | 25.76 |
| ATOM | 1009 | OH  | TYR | A | 130 | 13.899 | 55.864 | 54.894 | 1.00 | 40.52 |
| ATOM | 1010 | N   | LEU | A | 131 | 7.832  | 57.842 | 54.647 | 1.00 | 31.12 |
| ATOM | 1011 | CA  | LEU | A | 131 | 6.994  | 56.868 | 55.303 | 1.00 | 30.43 |
| ATOM | 1012 | C   | LEU | A | 131 | 7.691  | 55.568 | 55.289 | 1.00 | 33.91 |
| ATOM | 1013 | O   | LEU | A | 131 | 8.398  | 55.257 | 54.397 | 1.00 | 33.68 |
| ATOM | 1014 | CB  | LEU | A | 131 | 5.679  | 56.761 | 54.530 | 1.00 | 26.16 |
| ATOM | 1015 | CG  | LEU | A | 131 | 5.065  | 55.367 | 54.600 | 1.00 | 21.68 |
| ATOM | 1016 | CD1 | LEU | A | 131 | 4.163  | 55.206 | 55.797 | 1.00 | 17.56 |
| ATOM | 1017 | CD2 | LEU | A | 131 | 4.222  | 55.008 | 53.380 | 1.00 | 13.86 |
| ATOM | 1018 | N   | PHE | A | 132 | 7.533  | 54.828 | 56.348 | 1.00 | 29.24 |
| ATOM | 1019 | CA  | PHE | A | 132 | 8.129  | 53.527 | 56.323 | 1.00 | 33.44 |
| ATOM | 1020 | C   | PHE | A | 132 | 7.299  | 52.519 | 57.157 | 1.00 | 41.08 |
| ATOM | 1021 | O   | PHE | A | 132 | 6.344  | 52.889 | 57.837 | 1.00 | 46.05 |
| ATOM | 1022 | CB  | PHE | A | 132 | 9.621  | 53.670 | 56.791 | 1.00 | 36.40 |
| ATOM | 1023 | CG  | PHE | A | 132 | 9.763  | 53.895 | 58.256 | 1.00 | 38.11 |
| ATOM | 1024 | CD1 | PHE | A | 132 | 9.601  | 52.821 | 59.053 | 1.00 | 37.18 |
| ATOM | 1025 | CD2 | PHE | A | 132 | 10.123 | 55.158 | 58.803 | 1.00 | 43.89 |
| ATOM | 1026 | CE1 | PHE | A | 132 | 9.771  | 52.936 | 60.422 | 1.00 | 41.04 |
| ATOM | 1027 | CE2 | PHE | A | 132 | 10.289 | 55.258 | 60.174 | 1.00 |       |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 1046 | C   | CYS | A | 135 | 5.442  | 43.006 | 60.662 | 1.00 | 39.58 |
| ATOM | 1047 | O   | CYS | A | 135 | 4.597  | 42.144 | 60.739 | 1.00 | 40.94 |
| ATOM | 1048 | CB  | CYS | A | 135 | 5.098  | 43.794 | 58.320 | 1.00 | 35.40 |
| ATOM | 1049 | SG  | CYS | A | 135 | 3.976  | 44.922 | 57.445 | 1.00 | 41.22 |
| ATOM | 1050 | N   | GLN | A | 136 | 6.582  | 42.949 | 61.345 | 1.00 | 37.37 |
| ATOM | 1051 | CA  | GLN | A | 136 | 6.715  | 41.982 | 62.417 | 1.00 | 35.71 |
| ATOM | 1052 | C   | GLN | A | 136 | 6.589  | 42.645 | 63.797 | 1.00 | 31.90 |
| ATOM | 1053 | O   | GLN | A | 136 | 6.878  | 43.803 | 63.981 | 1.00 | 30.54 |
| ATOM | 1054 | CB  | GLN | A | 136 | 8.077  | 41.311 | 62.295 | 1.00 | 37.24 |
| ATOM | 1055 | CG  | GLN | A | 136 | 8.076  | 39.878 | 62.847 | 1.00 | 29.70 |
| ATOM | 1056 | CD  | GLN | A | 136 | 9.483  | 39.511 | 63.235 | 1.00 | 36.48 |
| ATOM | 1057 | OE1 | GLN | A | 136 | 10.366 | 40.328 | 63.356 | 1.00 | 24.49 |
| ATOM | 1058 | NE2 | GLN | A | 136 | 9.665  | 38.201 | 63.443 | 1.00 | 22.19 |
| ATOM | 1059 | N   | ALA | A | 137 | 5.850  | 41.899 | 64.648 | 1.00 | 28.56 |
| ATOM | 1060 | CA  | ALA | A | 137 | 5.235  | 40.581 | 64.351 | 1.00 | 28.89 |
| ATOM | 1061 | C   | ALA | A | 137 | 3.860  | 40.503 | 63.630 | 1.00 | 31.83 |
| ATOM | 1062 | O   | ALA | A | 137 | 3.679  | 39.688 | 62.738 | 1.00 | 29.67 |
| ATOM | 1063 | CB  | ALA | A | 137 | 5.091  | 39.742 | 65.625 | 1.00 | 28.91 |
| ATOM | 1064 | N   | ILE | A | 138 | 2.863  | 41.285 | 64.070 | 1.00 | 27.07 |
| ATOM | 1065 | CA  | ILE | A | 138 | 1.553  | 41.176 | 63.445 | 1.00 | 23.90 |
| ATOM | 1066 | C   | ILE | A | 138 | 0.960  | 42.492 | 63.053 | 1.00 | 28.69 |
| ATOM | 1067 | O   | ILE | A | 138 | -0.144 | 42.822 | 63.426 | 1.00 | 31.92 |
| ATOM | 1068 | CB  | ILE | A | 138 | 0.641  | 40.357 | 64.339 | 1.00 | 25.41 |
| ATOM | 1069 | CG1 | ILE | A | 138 | 0.871  | 40.811 | 65.801 | 1.00 | 27.32 |
| ATOM | 1070 | CG2 | ILE | A | 138 | 1.162  | 38.938 | 64.191 | 1.00 | 16.34 |
| ATOM | 1071 | CD1 | ILE | A | 138 | -0.275 | 40.615 | 66.826 | 1.00 | 20.22 |
| ATOM | 1072 | N   | HIS | A | 139 | 1.718  | 43.223 | 62.265 | 1.00 | 24.05 |
| ATOM | 1073 | CA  | HIS | A | 139 | 1.322  | 44.511 | 61.824 | 1.00 | 24.05 |
| ATOM | 1074 | C   | HIS | A | 139 | 0.982  | 44.579 | 60.351 | 1.00 | 34.40 |
| ATOM | 1075 | O   | HIS | A | 139 | 0.539  | 45.625 | 59.888 | 1.00 | 35.89 |
| ATOM | 1076 | CB  | HIS | A | 139 | 2.439  | 45.519 | 62.173 | 1.00 | 24.63 |
| ATOM | 1077 | CG  | HIS | A | 139 | 2.689  | 45.619 | 63.657 | 1.00 | 27.97 |
| ATOM | 1078 | ND1 | HIS | A | 139 | 1.679  | 45.970 | 64.571 | 1.00 | 27.75 |
| ATOM | 1079 | CD2 | HIS | A | 139 | 3.835  | 45.437 | 64.356 | 1.00 | 28.42 |
| ATOM | 1080 | CE1 | HIS | A | 139 | 2.222  | 45.983 | 65.770 | 1.00 | 26.19 |
| ATOM | 1081 | NE2 | HIS | A | 139 | 3.517  | 45.668 | 65.671 | 1.00 | 27.42 |
| ATOM | 1082 | N   | CYS | A | 140 | 1.181  | 43.490 | 59.598 | 1.00 | 30.28 |
| ATOM | 1083 | CA  | CYS | A | 140 | 0.832  | 43.517 | 58.181 | 1.00 | 28.08 |
| ATOM | 1084 | C   | CYS | A | 140 | -0.671 | 43.765 | 58.011 | 1.00 | 28.98 |
| ATOM | 1085 | O   | CYS | A | 140 | -1.111 | 44.449 | 57.066 | 1.00 | 30.00 |
| ATOM | 1086 | CB  | CYS | A | 140 | 1.181  | 42.213 | 57.447 | 1.00 | 28.82 |
| ATOM | 1087 | SG  | CYS | A | 140 | 1.330  | 42.483 | 55.661 | 1.00 | 34.37 |
| ATOM | 1088 | N   | ARG | A | 141 | -1.440 | 43.168 | 58.949 | 1.00 | 20.78 |
| ATOM | 1089 | CA  | ARG | A | 141 | -2.884 | 43.252 | 58.996 | 1.00 | 20.33 |
| ATOM | 1090 | C   | ARG | A | 141 | -3.286 | 44.684 | 59.003 | 1.00 | 32.37 |
| ATOM | 1091 | O   | ARG | A | 141 | -4.355 | 45.032 | 58.510 | 1.00 | 35.81 |
| ATOM | 1092 | CB  | ARG | A | 141 | -3.557 | 42.498 | 60.156 | 1.00 | 14.60 |
| ATOM | 1093 | CG  | ARG | A | 141 | -3.081 | 42.891 | 61.568 | 1.00 | 20.94 |
| ATOM | 1094 | CD  | ARG | A | 141 | -3.576 | 41.978 | 62.715 | 1.00 | 19.99 |
| ATOM | 1095 | NE  | ARG | A | 141 | -2.911 | 40.690 | 62.786 | 1.00 | 18.24 |
| ATOM | 1096 | CZ  | ARG | A | 141 | -3.140 | 39.707 | 63.648 | 1.00 | 18.77 |
| ATOM | 1097 | NH1 | ARG | A | 141 | -4.029 | 39.739 | 64.634 | 1.00 | 20.76 |
| ATOM | 1098 | NH2 | ARG | A | 141 | -2.415 | 38.640 | 63.508 | 1.00 | 24.20 |
| ATOM | 1099 | N   | ALA | A | 142 | -2.408 | 45.511 | 59.580 | 1.00 | 28.35 |
| ATOM | 1100 | CA  | ALA | A | 142 | -2.668 | 46.940 | 59.657 | 1.00 | 27.60 |
| ATOM | 1101 | C   | ALA | A | 142 | -2.369 | 47.652 | 58.345 | 1.00 | 34.33 |
| ATOM | 1102 | O   | ALA | A | 142 | -2.620 | 48.835 | 58.203 | 1.00 | 34.36 |
| ATOM | 1103 | CB  | ALA | A | 142 | -1.994 | 47.616 | 60.843 | 1.00 | 27.67 |
| ATOM | 1104 | N   | ILE | A | 143 | -1.824 | 46.922 | 57.382 | 1.00 | 32.39 |
| ATOM | 1105 | CA  | ILE | A | 143 | -1.537 | 47.499 | 56.099 | 1.00 | 30.38 |
| ATOM | 1106 | C   | ILE | A | 143 | -2.520 | 46.994 | 55.067 | 1.00 | 37.79 |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 1107 | O   | ILE | A | 143 | -2.885 | 47.709 | 54.152 | 1.00 | 42.65 |
| ATOM | 1108 | CB  | ILE | A | 143 | -0.142 | 47.228 | 55.613 | 1.00 | 32.06 |
| ATOM | 1109 | CG1 | ILE | A | 143 | 0.827  | 48.062 | 56.414 | 1.00 | 31.71 |
| ATOM | 1110 | CG2 | ILE | A | 143 | -0.074 | 47.654 | 54.143 | 1.00 | 34.02 |
| ATOM | 1111 | CD1 | ILE | A | 143 | 2.258  | 47.774 | 55.988 | 1.00 | 42.10 |
| ATOM | 1112 | N   | LEU | A | 144 | -2.939 | 45.749 | 55.218 | 1.00 | 32.50 |
| ATOM | 1113 | CA  | LEU | A | 144 | -3.873 | 45.142 | 54.291 | 1.00 | 32.36 |
| ATOM | 1114 | C   | LEU | A | 144 | -4.435 | 43.838 | 54.849 | 1.00 | 40.36 |
| ATOM | 1115 | O   | LEU | A | 144 | -3.959 | 43.278 | 55.852 | 1.00 | 33.27 |
| ATOM | 1116 | CB  | LEU | A | 144 | -3.250 | 44.936 | 52.894 | 1.00 | 31.58 |
| ATOM | 1117 | CG  | LEU | A | 144 | -1.923 | 44.170 | 52.917 | 1.00 | 33.31 |
| ATOM | 1118 | CD1 | LEU | A | 144 | -2.147 | 42.770 | 52.352 | 1.00 | 32.07 |
| ATOM | 1119 | CD2 | LEU | A | 144 | -0.836 | 44.897 | 52.110 | 1.00 | 28.67 |
| ATOM | 1120 | N   | PRO | A | 145 | -5.490 | 43.347 | 54.213 | 1.00 | 40.02 |
| ATOM | 1121 | CA  | PRO | A | 145 | -6.080 | 42.129 | 54.715 | 1.00 | 37.86 |
| ATOM | 1122 | C   | PRO | A | 145 | -5.264 | 40.941 | 54.286 | 1.00 | 37.87 |
| ATOM | 1123 | O   | PRO | A | 145 | -4.819 | 40.831 | 53.144 | 1.00 | 35.27 |
| ATOM | 1124 | CB  | PRO | A | 145 | -7.530 | 42.080 | 54.220 | 1.00 | 38.81 |
| ATOM | 1125 | CG  | PRO | A | 145 | -7.778 | 43.393 | 53.492 | 1.00 | 41.34 |
| ATOM | 1126 | CD  | PRO | A | 145 | -6.432 | 44.093 | 53.341 | 1.00 | 36.69 |
| ATOM | 1127 | N   | CYS | A | 146 | -5.041 | 40.056 | 55.233 | 1.00 | 36.18 |
| ATOM | 1128 | CA  | CYS | A | 146 | -4.250 | 38.882 | 54.958 | 1.00 | 35.60 |
| ATOM | 1129 | C   | CYS | A | 146 | -4.358 | 37.859 | 56.069 | 1.00 | 33.04 |
| ATOM | 1130 | O   | CYS | A | 146 | -5.067 | 38.062 | 57.050 | 1.00 | 30.78 |
| ATOM | 1131 | CB  | CYS | A | 146 | -2.761 | 39.287 | 54.813 | 1.00 | 36.08 |
| ATOM | 1132 | SG  | CYS | A | 146 | -2.087 | 40.108 | 56.302 | 1.00 | 39.43 |
| ATOM | 1133 | N   | GLN | A | 147 | -3.637 | 36.755 | 55.883 | 1.00 | 29.33 |
| ATOM | 1134 | CA  | GLN | A | 147 | -3.517 | 35.703 | 56.875 | 1.00 | 29.71 |
| ATOM | 1135 | C   | GLN | A | 147 | -2.254 | 36.131 | 57.628 | 1.00 | 38.75 |
| ATOM | 1136 | O   | GLN | A | 147 | -1.141 | 35.926 | 57.135 | 1.00 | 40.79 |
| ATOM | 1137 | CB  | GLN | A | 147 | -3.322 | 34.352 | 56.206 | 1.00 | 28.99 |
| ATOM | 1138 | CG  | GLN | A | 147 | -4.672 | 33.707 | 55.894 | 1.00 | 25.73 |
| ATOM | 1139 | CD  | GLN | A | 147 | -4.562 | 32.532 | 54.960 | 1.00 | 39.92 |
| ATOM | 1140 | OE1 | GLN | A | 147 | -4.217 | 32.668 | 53.775 | 1.00 | 43.89 |
| ATOM | 1141 | NE2 | GLN | A | 147 | -4.828 | 31.368 | 55.499 | 1.00 | 26.36 |
| ATOM | 1142 | N   | ASP | A | 148 | -2.425 | 36.834 | 58.765 | 1.00 | 32.68 |
| ATOM | 1143 | CA  | ASP | A | 148 | -1.287 | 37.362 | 59.474 | 1.00 | 33.50 |
| ATOM | 1144 | C   | ASP | A | 148 | -0.629 | 36.377 | 60.371 | 1.00 | 33.13 |
| ATOM | 1145 | O   | ASP | A | 148 | -0.622 | 36.563 | 61.584 | 1.00 | 31.30 |
| ATOM | 1146 | CB  | ASP | A | 148 | -1.633 | 38.642 | 60.253 | 1.00 | 37.78 |
| ATOM | 1147 | CG  | ASP | A | 148 | -0.535 | 39.666 | 60.332 | 1.00 | 45.10 |
| ATOM | 1148 | OD1 | ASP | A | 148 | 0.564  | 39.540 | 59.836 | 1.00 | 47.89 |
| ATOM | 1149 | OD2 | ASP | A | 148 | -0.913 | 40.737 | 60.952 | 1.00 | 48.63 |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 1168 | CB  | SER | A | 151 | 1.714  | 29.203 | 59.905 | 1.00 | 25.95 |
| ATOM | 1169 | OG  | SER | A | 151 | 0.483  | 29.685 | 59.439 | 1.00 | 49.35 |
| ATOM | 1170 | N   | VAL | A | 152 | 1.997  | 30.887 | 57.024 | 1.00 | 34.36 |
| ATOM | 1171 | CA  | VAL | A | 152 | 1.595  | 31.015 | 55.623 | 1.00 | 33.74 |
| ATOM | 1172 | C   | VAL | A | 152 | 2.705  | 31.764 | 54.847 | 1.00 | 37.45 |
| ATOM | 1173 | O   | VAL | A | 152 | 3.295  | 32.761 | 55.313 | 1.00 | 37.63 |
| ATOM | 1174 | CB  | VAL | A | 152 | 0.203  | 31.697 | 55.427 | 1.00 | 32.61 |
| ATOM | 1175 | CG1 | VAL | A | 152 | -0.184 | 31.767 | 53.963 | 1.00 | 31.50 |
| ATOM | 1176 | CG2 | VAL | A | 152 | -0.915 | 30.975 | 56.149 | 1.00 | 31.29 |
| ATOM | 1177 | N   | LYS | A | 153 | 2.999  | 31.289 | 53.654 | 1.00 | 26.98 |
| ATOM | 1178 | CA  | LYS | A | 153 | 4.002  | 31.927 | 52.866 | 1.00 | 25.81 |
| ATOM | 1179 | C   | LYS | A | 153 | 3.469  | 32.141 | 51.473 | 1.00 | 33.94 |
| ATOM | 1180 | O   | LYS | A | 153 | 2.826  | 31.251 | 50.936 | 1.00 | 32.91 |
| ATOM | 1181 | CB  | LYS | A | 153 | 5.252  | 31.091 | 52.841 | 1.00 | 24.70 |
| ATOM | 1182 | CG  | LYS | A | 153 | 6.383  | 31.760 | 53.583 | 1.00 | 34.68 |
| ATOM | 1183 | CD  | LYS | A | 153 | 7.641  | 30.893 | 53.616 | 1.00 | 39.37 |
| ATOM | 1184 | CE  | LYS | A | 153 | 8.121  | 30.506 | 55.015 | 1.00 | 29.09 |
| ATOM | 1185 | NZ  | LYS | A | 153 | 9.556  | 30.152 | 55.112 | 1.00 | 26.03 |
| ATOM | 1186 | N   | LEU | A | 154 | 3.732  | 33.321 | 50.896 | 1.00 | 32.13 |
| ATOM | 1187 | CA  | LEU | A | 154 | 3.285  | 33.639 | 49.544 | 1.00 | 30.67 |
| ATOM | 1188 | C   | LEU | A | 154 | 4.279  | 34.475 | 48.789 | 1.00 | 40.67 |
| ATOM | 1189 | O   | LEU | A | 154 | 5.264  | 35.000 | 49.344 | 1.00 | 42.56 |
| ATOM | 1190 | CB  | LEU | A | 154 | 1.966  | 34.432 | 49.515 | 1.00 | 30.10 |
| ATOM | 1191 | CG  | LEU | A | 154 | 2.084  | 35.793 | 50.207 | 1.00 | 35.20 |
| ATOM | 1192 | CD1 | LEU | A | 154 | 0.989  | 36.716 | 49.690 | 1.00 | 37.21 |
| ATOM | 1193 | CD2 | LEU | A | 154 | 1.934  | 35.608 | 51.715 | 1.00 | 33.07 |
| ATOM | 1194 | N   | THR | A | 155 | 3.963  | 34.610 | 47.499 | 1.00 | 37.82 |
| ATOM | 1195 | CA  | THR | A | 155 | 4.728  | 35.449 | 46.596 | 1.00 | 38.44 |
| ATOM | 1196 | C   | THR | A | 155 | 3.934  | 36.730 | 46.389 | 1.00 | 41.52 |
| ATOM | 1197 | O   | THR | A | 155 | 2.738  | 36.775 | 46.674 | 1.00 | 43.95 |
| ATOM | 1198 | CB  | THR | A | 155 | 5.041  | 34.814 | 45.230 | 1.00 | 36.99 |
| ATOM | 1199 | OG1 | THR | A | 155 | 3.886  | 34.281 | 44.584 | 1.00 | 32.59 |
| ATOM | 1200 | CG2 | THR | A | 155 | 6.133  | 33.790 | 45.404 | 1.00 | 18.24 |
| ATOM | 1201 | N   | TYR | A | 156 | 4.563  | 37.768 | 45.892 | 1.00 | 33.87 |
| ATOM | 1202 | CA  | TYR | A | 156 | 3.835  | 39.003 | 45.683 | 1.00 | 32.49 |
| ATOM | 1203 | C   | TYR | A | 156 | 4.509  | 39.922 | 44.717 | 1.00 | 37.91 |
| ATOM | 1204 | O   | TYR | A | 156 | 5.725  | 39.940 | 44.562 | 1.00 | 39.04 |
| ATOM | 1205 | CB  | TYR | A | 156 | 3.534  | 39.795 | 46.983 | 1.00 | 31.16 |
| ATOM | 1206 | CG  | TYR | A | 156 | 4.642  | 40.731 | 47.471 | 1.00 | 28.94 |
| ATOM | 1207 | CD1 | TYR | A | 156 | 4.817  | 42.021 | 46.969 | 1.00 | 30.33 |
| ATOM | 1208 | CD2 | TYR | A | 156 | 5.525  | 40.303 | 48.465 | 1.00 | 30.43 |
| ATOM | 1209 | CE1 | TYR | A | 156 | 5.829  | 42.853 | 47.459 | 1.00 | 36.89 |
| ATOM | 1210 | CE2 | TYR | A | 156 | 6.553  | 41.104 | 48.960 | 1.00 |       |







|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
|    | ATOM | 3059 | N   | LEU | A | 390 | 22.374 | 27.059 | 71.172 | 1.00 | 11.37 |
|    | ATOM | 3060 | CA  | LEU | A | 390 | 23.140 | 26.650 | 69.998 | 1.00 | 9.78  |
|    | ATOM | 3061 | C   | LEU | A | 390 | 24.651 | 26.539 | 70.251 | 1.00 | 19.70 |
|    | ATOM | 3062 | O   | LEU | A | 390 | 25.305 | 25.609 | 69.745 | 1.00 | 18.74 |
| 5  | ATOM | 3063 | CB  | LEU | A | 390 | 22.887 | 27.525 | 68.764 | 1.00 | 9.94  |
|    | ATOM | 3064 | CG  | LEU | A | 390 | 21.402 | 27.590 | 68.367 | 1.00 | 14.32 |
|    | ATOM | 3065 | CD1 | LEU | A | 390 | 21.153 | 28.632 | 67.257 | 1.00 | 14.04 |
|    | ATOM | 3066 | CD2 | LEU | A | 390 | 20.902 | 26.209 | 67.923 | 1.00 | 14.70 |
| 10 | ATOM | 3067 | N   | PHE | A | 391 | 25.205 | 27.490 | 71.026 | 1.00 | 12.66 |
|    | ATOM | 3068 | CA  | PHE | A | 391 | 26.635 | 27.538 | 71.333 | 1.00 | 13.86 |
|    | ATOM | 3069 | C   | PHE | A | 391 | 27.053 | 26.343 | 72.147 | 1.00 | 17.87 |
|    | ATOM | 3070 | O   | PHE | A | 391 | 28.104 | 25.733 | 71.983 | 1.00 | 18.52 |
|    | ATOM | 3071 | CB  | PHE | A | 391 | 26.964 | 28.806 | 72.105 | 1.00 | 14.47 |
|    | ATOM | 3072 | CG  | PHE | A | 391 | 28.437 | 29.179 | 72.101 | 1.00 | 18.51 |
| 15 | ATOM | 3073 | CD1 | PHE | A | 391 | 29.237 | 28.996 | 70.973 | 1.00 | 18.55 |
|    | ATOM | 3074 | CD2 | PHE | A | 391 | 29.030 | 29.748 | 73.233 | 1.00 | 18.59 |
|    | ATOM | 3075 | CE1 | PHE | A | 391 | 30.571 | 29.402 | 70.966 | 1.00 | 15.73 |
|    | ATOM | 3076 | CE2 | PHE | A | 391 | 30.373 | 30.137 | 73.252 | 1.00 | 18.49 |
| 20 | ATOM | 3077 | CZ  | PHE | A | 391 | 31.148 | 29.954 | 72.109 | 1.00 | 15.63 |
|    | ATOM | 3078 | N   | TYR | A | 392 | 26.148 | 26.008 | 73.039 | 1.00 | 16.91 |
|    | ATOM | 3079 | CA  | TYR | A | 392 | 26.315 | 24.893 | 73.944 | 1.00 | 17.78 |
|    | ATOM | 3080 | C   | TYR | A | 392 | 26.288 | 23.570 | 73.175 | 1.00 | 19.46 |
|    | ATOM | 3081 | O   | TYR | A | 392 | 27.095 | 22.666 | 73.388 | 1.00 | 18.21 |
| 25 | ATOM | 3082 | CB  | TYR | A | 392 | 25.243 | 25.000 | 75.049 | 1.00 | 15.50 |
|    | ATOM | 3083 | CG  | TYR | A | 392 | 24.928 | 23.688 | 75.736 | 1.00 | 20.94 |
|    | ATOM | 3084 | CD1 | TYR | A | 392 | 25.849 | 23.106 | 76.609 | 1.00 | 24.90 |
|    | ATOM | 3085 | CD2 | TYR | A | 392 | 23.715 | 23.034 | 75.528 | 1.00 | 21.37 |
|    | ATOM | 3086 | CE1 | TYR | A | 392 | 25.596 | 21.899 | 77.260 | 1.00 | 23.89 |
|    | ATOM | 3087 | CE2 | TYR | A | 392 | 23.438 | 21.821 | 76.162 | 1.00 | 24.11 |
| 30 | ATOM | 3088 | CZ  | TYR | A | 392 | 24.383 | 21.256 | 77.020 | 1.00 | 28.03 |
|    | ATOM | 3089 | OH  | TYR | A | 392 | 24.112 | 20.087 | 77.665 | 1.00 | 20.09 |
|    | ATOM | 3090 | N   | LEU | A | 393 | 25.332 | 23.456 | 72.271 | 1.00 | 14.83 |
|    | ATOM | 3091 | CA  | LEU | A | 393 | 25.210 | 22.267 | 71.440 | 1.00 | 15.47 |
| 35 | ATOM | 3092 | C   | LEU | A | 393 | 26.432 | 22.122 | 70.544 | 1.00 | 20.32 |
|    | ATOM | 3093 | O   | LEU | A | 393 | 26.867 | 21.005 | 70.304 | 1.00 | 21.36 |
|    | ATOM | 3094 | CB  | LEU | A | 393 | 23.961 | 22.344 | 70.508 | 1.00 | 16.00 |
|    | ATOM | 3095 | CG  | LEU | A | 393 | 22.638 | 22.027 | 71.223 | 1.00 | 18.37 |
|    | ATOM | 3096 | CD1 | LEU | A | 393 | 21.443 | 22.392 | 70.347 | 1.00 | 15.16 |
| 40 | ATOM | 3097 | CD2 | LEU | A | 393 | 22.577 | 20.601 | 71.795 | 1.00 | 17.06 |
|    | ATOM | 3098 | N   | GLU | A | 394 | 26.921 | 23.255 | 70.015 | 1.00 | 16.00 |
|    | ATOM | 3099 | CA  | GLU | A | 394 | 28.104 | 23.298 | 69.160 | 1.00 | 13.58 |
|    | ATOM | 3100 | C   | GLU | A | 394 | 29.268 | 22.719 | 69.931 | 1.00 | 17.05 |
|    | ATOM | 3101 | O   | GLU | A | 394 | 30.014 | 21.889 | 69.453 | 1.00 | 15.79 |
| 45 | ATOM | 3102 | CB  | GLU | A | 394 | 28.434 | 24.745 | 68.776 | 1.00 | 17.59 |
|    | ATOM | 3103 | CG  | GLU | A | 394 | 29.903 | 24.871 | 68.320 | 1.00 | 23.24 |
|    | ATOM | 3104 | CD  | GLU | A | 394 | 30.332 | 26.300 | 68.152 | 1.00 | 32.12 |
|    | ATOM | 3105 | OE1 | GLU | A | 394 | 29.709 | 27.146 | 67.532 | 1.00 | 23.57 |
|    | ATOM | 3106 | OE2 | GLU | A | 394 | 31.480 | 26.547 | 68.714 | 1.00 | 26.27 |
| 50 | ATOM | 3107 | N   | GLN | A | 395 | 29.410 | 23.127 | 71.183 | 1.00 | 16.99 |
|    | ATOM | 3108 | CA  | GLN | A | 395 | 30.462 | 22.610 | 72.030 | 1.00 | 17.56 |
|    | ATOM | 3109 | C   | GLN | A | 395 | 30.293 | 21.127 | 72.360 | 1.00 | 23.89 |
|    | ATOM | 3110 | O   | GLN | A | 395 | 31.258 | 20.359 | 72.421 | 1.00 | 24.66 |
|    | ATOM | 3111 | CB  | GLN | A | 395 | 30.725 | 23.461 | 73.318 | 1.00 | 17.71 |
| 55 | ATOM | 3112 | CG  | GLN | A | 395 | 31.195 | 24.888 | 72.918 | 1.00 | 17.45 |
|    | ATOM | 3113 | CD  | GLN | A | 395 | 31.354 | 25.851 | 74.081 | 1.00 | 21.98 |
|    | ATOM | 3114 | OE1 | GLN | A | 395 | 30.986 | 25.584 | 75.224 | 1.00 | 16.80 |
|    | ATOM | 3115 | NE2 | GLN | A | 395 | 31.943 | 26.985 | 73.776 | 1.00 | 16.78 |
|    | ATOM | 3116 | N   | LEU | A | 396 | 29.058 | 20.706 | 72.588 | 1.00 | 21.86 |
| 60 | ATOM | 3117 | CA  | LEU | A | 396 | 28.767 | 19.330 | 72.932 | 1.00 | 20.27 |
|    | ATOM | 3118 | C   | LEU | A | 396 | 28.936 | 18.387 | 71.744 | 1.00 | 22.03 |
|    | ATOM | 3119 | O   | LEU | A | 396 | 29.381 | 17.260 | 71.857 | 1.00 | 25.07 |
|    | ATOM | 3120 | CB  | LEU | A | 396 | 27.315 | 19.276 | 73.441 | 1.00 | 18.56 |
|    | ATOM | 3121 | CG  | LEU | A | 396 | 26.852 | 17.960 | 73.994 | 1.00 | 22.66 |
|    | ATOM | 3122 | CD1 | LEU | A | 396 | 27.493 | 17.780 | 75.354 | 1.00 | 25.52 |



|    |      |      |     |     |   |     |        |        |        |      |        |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
|    | ATOM | 3123 | CD2 | LEU | A | 396 | 25.340 | 18.045 | 74.179 | 1.00 | 17.79  |
|    | ATOM | 3124 | N   | LEU | A | 397 | 28.575 | 18.831 | 70.579 | 1.00 | 15.28  |
|    | ATOM | 3125 | CA  | LEU | A | 397 | 28.603 | 17.939 | 69.433 | 1.00 | 16.80  |
| 5  | ATOM | 3126 | C   | LEU | A | 397 | 29.846 | 17.946 | 68.565 | 1.00 | 26.85  |
|    | ATOM | 3127 | O   | LEU | A | 397 | 29.864 | 17.399 | 67.458 | 1.00 | 29.08  |
|    | ATOM | 3128 | CB  | LEU | A | 397 | 27.371 | 18.242 | 68.552 | 1.00 | 15.51  |
|    | ATOM | 3129 | CG  | LEU | A | 397 | 26.013 | 18.018 | 69.261 | 1.00 | 20.96  |
|    | ATOM | 3130 | CD1 | LEU | A | 397 | 24.874 | 18.717 | 68.501 | 1.00 | 19.35  |
| 10 | ATOM | 3131 | CD2 | LEU | A | 397 | 25.692 | 16.536 | 69.461 | 1.00 | 19.12  |
|    | ATOM | 3132 | N   | GLY | A | 398 | 30.901 | 18.598 | 68.985 | 1.00 | 24.55  |
|    | ATOM | 3133 | CA  | GLY | A | 398 | 32.006 | 18.516 | 68.076 | 1.00 | 27.19  |
|    | ATOM | 3134 | C   | GLY | A | 398 | 32.648 | 19.794 | 67.598 | 1.00 | 29.41  |
|    | ATOM | 3135 | O   | GLY | A | 398 | 33.743 | 19.713 | 67.048 | 1.00 | 30.13  |
| 15 | ATOM | 3136 | N   | GLY | A | 399 | 32.020 | 20.951 | 67.752 | 1.00 | 19.25  |
|    | ATOM | 3137 | CA  | GLY | A | 399 | 32.700 | 22.143 | 67.291 | 1.00 | 16.50  |
|    | ATOM | 3138 | C   | GLY | A | 399 | 31.937 | 22.850 | 66.212 | 1.00 | 15.03  |
|    | ATOM | 3139 | O   | GLY | A | 399 | 30.976 | 22.315 | 65.694 | 1.00 | 17.49  |
|    | ATOM | 3140 | N   | PRO | A | 400 | 32.397 | 24.045 | 65.870 | 1.00 | 21.52  |
| 20 | ATOM | 3141 | CA  | PRO | A | 400 | 31.758 | 24.918 | 64.909 | 1.00 | 21.69  |
|    | ATOM | 3142 | C   | PRO | A | 400 | 31.599 | 24.312 | 63.552 | 1.00 | 29.85  |
|    | ATOM | 3143 | O   | PRO | A | 400 | 30.540 | 24.433 | 62.921 | 1.00 | 24.28  |
|    | ATOM | 3144 | CB  | PRO | A | 400 | 32.574 | 26.210 | 64.802 | 1.00 | 21.33  |
|    | ATOM | 3145 | CG  | PRO | A | 400 | 33.868 | 25.949 | 65.552 | 1.00 | 27.07  |
| 25 | ATOM | 3146 | CD  | PRO | A | 400 | 33.698 | 24.635 | 66.306 | 1.00 | 25.67  |
|    | ATOM | 3147 | N   | GLU | A | 401 | 32.679 | 23.674 | 63.128 | 1.00 | 28.84  |
|    | ATOM | 3148 | CA  | GLU | A | 401 | 32.630 | 23.048 | 61.831 | 1.00 | 30.42  |
|    | ATOM | 3149 | C   | GLU | A | 401 | 31.491 | 22.055 | 61.764 | 1.00 | 22.63  |
|    | ATOM | 3150 | O   | GLU | A | 401 | 30.664 | 22.034 | 60.872 | 1.00 | 21.35  |
| 30 | ATOM | 3151 | CB  | GLU | A | 401 | 33.915 | 22.247 | 61.648 | 1.00 | 35.39  |
|    | ATOM | 3152 | CG  | GLU | A | 401 | 35.125 | 23.160 | 61.445 | 1.00 | 70.34  |
|    | ATOM | 3153 | CD  | GLU | A | 401 | 35.978 | 22.574 | 60.355 | 1.00 | 100.00 |
|    | ATOM | 3154 | OE1 | GLU | A | 401 | 35.711 | 21.486 | 59.851 | 1.00 | 100.00 |
|    | ATOM | 3155 | OE2 | GLU | A | 401 | 37.013 | 23.329 | 60.026 | 1.00 | 100.00 |
| 35 | ATOM | 3156 | N   | ILE | A | 402 | 31.484 | 21.185 | 62.731 | 1.00 | 20.44  |
|    | ATOM | 3157 | CA  | ILE | A | 402 | 30.481 | 20.165 | 62.766 | 1.00 | 21.27  |
|    | ATOM | 3158 | C   | ILE | A | 402 | 29.082 | 20.761 | 62.895 | 1.00 | 26.84  |
|    | ATOM | 3159 | O   | ILE | A | 402 | 28.142 | 20.366 | 62.199 | 1.00 | 18.68  |
|    | ATOM | 3160 | CB  | ILE | A | 402 | 30.819 | 19.218 | 63.904 | 1.00 | 24.03  |
| 40 | ATOM | 3161 | CG1 | ILE | A | 402 | 31.974 | 18.299 | 63.503 | 1.00 | 23.45  |
|    | ATOM | 3162 | CG2 | ILE | A | 402 | 29.587 | 18.421 | 64.334 | 1.00 | 28.69  |
|    | ATOM | 3163 | CD1 | ILE | A | 402 | 32.370 | 17.396 | 64.665 | 1.00 | 26.57  |
|    | ATOM | 3164 | N   | PHE | A | 403 | 28.948 | 21.745 | 63.773 | 1.00 | 21.88  |
|    | ATOM | 3165 | CA  | PHE | A | 403 | 27.646 | 22.325 | 63.962 | 1.00 | 20.25  |
| 45 | ATOM | 3166 | C   | PHE | A | 403 | 27.149 | 23.152 | 62.802 | 1.00 | 20.90  |
|    | ATOM | 3167 | O   | PHE | A | 403 | 25.951 | 23.246 | 62.510 | 1.00 | 21.88  |
|    | ATOM | 3168 | CB  | PHE | A | 403 | 27.555 | 23.073 | 65.298 | 1.00 | 22.18  |
|    | ATOM | 3169 | CG  | PHE | A | 403 | 26.121 | 23.247 | 65.764 | 1.00 | 20.23  |
|    | ATOM | 3170 | CD1 | PHE | A | 403 | 25.411 | 22.189 | 66.331 | 1.00 | 21.99  |
| 50 | ATOM | 3171 | CD2 | PHE | A | 403 | 25.478 | 24.479 | 65.660 | 1.00 | 25.50  |
|    | ATOM | 3172 | CE1 | PHE | A | 403 | 24.106 | 22.345 | 66.801 | 1.00 | 23.07  |
|    | ATOM | 3173 | CE2 | PHE | A | 403 | 24.156 | 24.651 | 66.081 | 1.00 | 25.44  |
|    | ATOM | 3174 | CZ  | PHE | A | 403 | 23.472 | 23.581 | 66.661 | 1.00 | 22.55  |
|    | ATOM | 3175 | N   | LEU | A | 404 | 28.076 | 23.804 | 62.121 | 1.00 | 17.83  |
| 55 | ATOM | 3176 | CA  | LEU | A | 404 | 27.664 | 24.596 | 60.973 | 1.00 | 17.93  |
|    | ATOM | 3177 | C   | LEU | A | 404 | 27.136 | 23.666 | 59.868 | 1.00 | 24.59  |
|    | ATOM | 3178 | O   | LEU | A | 404 | 26.297 | 24.031 | 59.044 | 1.00 | 22.86  |
|    | ATOM | 3179 | CB  | LEU | A | 404 | 28.808 | 25.526 | 60.504 | 1.00 | 17.59  |
|    | ATOM | 3180 | CG  | LEU | A | 404 | 28.952 | 26.728 | 61.425 | 1.00 | 19.68  |
| 60 | ATOM | 3181 | CD1 | LEU | A | 404 | 30.297 | 27.424 | 61.239 | 1.00 | 19.60  |
|    | ATOM | 3182 | CD2 | LEU | A | 404 | 27.873 | 27.719 | 61.047 | 1.00 | 20.62  |
|    | ATOM | 3183 | N   | GLY | A | 405 | 27.630 | 22.418 | 59.852 | 1.00 | 21.24  |
|    | ATOM | 3184 | CA  | GLY | A | 405 | 27.164 | 21.461 | 58.868 | 1.00 | 18.72  |
|    | ATOM | 3185 | C   | GLY | A | 405 | 25.691 | 21.148 | 59.148 | 1.00 | 23.90  |
|    | ATOM | 3186 | O   | GLY | A | 405 | 24.853 | 21.054 | 58.240 | 1.00 | 24.54  |



|    |      |      |     |     |   |     |        |        |        |      |        |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
|    | ATOM | 3187 | N   | PHE | A | 406 | 25.363 | 20.987 | 60.438 | 1.00 | 18.59  |
|    | ATOM | 3188 | CA  | PHE | A | 406 | 23.979 | 20.734 | 60.824 | 1.00 | 18.47  |
|    | ATOM | 3189 | C   | PHE | A | 406 | 23.165 | 21.964 | 60.367 | 1.00 | 23.08  |
| 5  | ATOM | 3190 | O   | PHE | A | 406 | 22.150 | 21.917 | 59.663 | 1.00 | 20.15  |
|    | ATOM | 3191 | CB  | PHE | A | 406 | 23.863 | 20.473 | 62.348 | 1.00 | 17.79  |
|    | ATOM | 3192 | CG  | PHE | A | 406 | 22.470 | 20.814 | 62.819 | 1.00 | 19.42  |
|    | ATOM | 3193 | CD1 | PHE | A | 406 | 21.400 | 19.986 | 62.482 | 1.00 | 20.66  |
|    | ATOM | 3194 | CD2 | PHE | A | 406 | 22.213 | 21.990 | 63.526 | 1.00 | 20.37  |
| 10 | ATOM | 3195 | CE1 | PHE | A | 406 | 20.099 | 20.274 | 62.898 | 1.00 | 22.34  |
|    | ATOM | 3196 | CE2 | PHE | A | 406 | 20.921 | 22.313 | 63.938 | 1.00 | 24.74  |
|    | ATOM | 3197 | CZ  | PHE | A | 406 | 19.874 | 21.441 | 63.634 | 1.00 | 23.87  |
|    | ATOM | 3198 | N   | LEU | A | 407 | 23.674 | 23.139 | 60.702 | 1.00 | 22.33  |
|    | ATOM | 3199 | CA  | LEU | A | 407 | 22.979 | 24.352 | 60.309 | 1.00 | 26.37  |
|    | ATOM | 3200 | C   | LEU | A | 407 | 22.690 | 24.501 | 58.819 | 1.00 | 24.88  |
| 15 | ATOM | 3201 | O   | LEU | A | 407 | 21.588 | 24.869 | 58.409 | 1.00 | 21.77  |
|    | ATOM | 3202 | CB  | LEU | A | 407 | 23.742 | 25.574 | 60.831 | 1.00 | 30.18  |
|    | ATOM | 3203 | CG  | LEU | A | 407 | 22.859 | 26.773 | 61.112 | 1.00 | 40.95  |
|    | ATOM | 3204 | CD1 | LEU | A | 407 | 23.559 | 27.710 | 62.083 | 1.00 | 43.78  |
|    | ATOM | 3205 | CD2 | LEU | A | 407 | 22.622 | 27.498 | 59.806 | 1.00 | 47.26  |
| 20 | ATOM | 3206 | N   | LYS | A | 408 | 23.679 | 24.256 | 57.981 | 1.00 | 21.87  |
|    | ATOM | 3207 | CA  | LYS | A | 408 | 23.425 | 24.378 | 56.555 | 1.00 | 20.93  |
|    | ATOM | 3208 | C   | LYS | A | 408 | 22.386 | 23.351 | 56.080 | 1.00 | 19.73  |
|    | ATOM | 3209 | O   | LYS | A | 408 | 21.502 | 23.596 | 55.265 | 1.00 | 18.85  |
| 25 | ATOM | 3210 | CB  | LYS | A | 408 | 24.715 | 24.325 | 55.746 | 1.00 | 22.33  |
|    | ATOM | 3211 | CG  | LYS | A | 408 | 24.420 | 24.240 | 54.262 | 1.00 | 33.19  |
|    | ATOM | 3212 | CD  | LYS | A | 408 | 25.621 | 24.508 | 53.374 | 1.00 | 24.21  |
|    | ATOM | 3213 | CE  | LYS | A | 408 | 26.812 | 25.035 | 54.131 | 1.00 | 44.20  |
|    | ATOM | 3214 | NZ  | LYS | A | 408 | 27.904 | 25.399 | 53.217 | 1.00 | 61.63  |
|    | ATOM | 3215 | N   | ALA | A | 409 | 22.458 | 22.161 | 56.625 | 1.00 | 21.49  |
| 30 | ATOM | 3216 | CA  | ALA | A | 409 | 21.496 | 21.116 | 56.278 | 1.00 | 23.64  |
|    | ATOM | 3217 | C   | ALA | A | 409 | 20.037 | 21.458 | 56.689 | 1.00 | 28.20  |
|    | ATOM | 3218 | O   | ALA | A | 409 | 19.059 | 21.204 | 55.968 | 1.00 | 23.25  |
|    | ATOM | 3219 | CB  | ALA | A | 409 | 21.936 | 19.821 | 56.974 | 1.00 | 23.41  |
|    | ATOM | 3220 | N   | TYR | A | 410 | 19.921 | 22.030 | 57.900 | 1.00 | 23.19  |
| 35 | ATOM | 3221 | CA  | TYR | A | 410 | 18.668 | 22.463 | 58.495 | 1.00 | 18.98  |
|    | ATOM | 3222 | C   | TYR | A | 410 | 18.014 | 23.507 | 57.594 | 1.00 | 18.81  |
|    | ATOM | 3223 | O   | TYR | A | 410 | 16.832 | 23.464 | 57.298 | 1.00 | 19.59  |
|    | ATOM | 3224 | CB  | TYR | A | 410 | 18.973 | 22.980 | 59.910 | 1.00 | 19.89  |
|    | ATOM | 3225 | CG  | TYR | A | 410 | 17.947 | 23.924 | 60.516 | 1.00 | 20.57  |
| 40 | ATOM | 3226 | CD1 | TYR | A | 410 | 16.715 | 23.463 | 60.981 | 1.00 | 22.20  |
|    | ATOM | 3227 | CD2 | TYR | A | 410 | 18.219 | 25.286 | 60.649 | 1.00 | 21.16  |
|    | ATOM | 3228 | CE1 | TYR | A | 410 | 15.767 | 24.320 | 61.551 | 1.00 | 17.85  |
|    | ATOM | 3229 | CE2 | TYR | A | 410 | 17.289 | 26.163 | 61.213 | 1.00 | 22.58  |
|    | ATOM | 3230 | CZ  | TYR | A | 410 | 16.064 | 25.679 | 61.682 | 1.00 | 25.33  |
| 45 | ATOM | 3231 | OH  | TYR | A | 410 | 15.182 | 26.528 | 62.315 | 1.00 | 20.84  |
|    | ATOM | 3232 | N   | VAL | A | 411 | 18.809 | 24.459 | 57.147 | 1.00 | 17.01  |
|    | ATOM | 3233 | CA  | VAL | A | 411 | 18.378 | 25.520 | 56.254 | 1.00 | 20.36  |
|    | ATOM | 3234 | C   | VAL | A | 411 | 17.876 | 24.946 | 54.936 | 1.00 | 25.04  |
|    | ATOM | 3235 | O   | VAL | A | 411 | 16.859 | 25.377 | 54.394 | 1.00 | 22.50  |
| 50 | ATOM | 3236 | CB  | VAL | A | 411 | 19.533 | 26.493 | 55.937 | 1.00 | 24.82  |
|    | ATOM | 3237 | CG1 | VAL | A | 411 | 19.220 | 27.380 | 54.724 | 1.00 | 21.10  |
|    | ATOM | 3238 | CG2 | VAL | A | 411 | 19.920 | 27.333 | 57.163 | 1.00 | 25.82  |
|    | ATOM | 3239 | N   | GLU | A | 412 | 18.616 | 23.952 | 54.443 | 1.00 | 24.87  |
|    | ATOM | 3240 | CA  | GLU | A | 412 | 18.264 | 23.283 | 53.202 | 1.00 | 24.91  |
| 55 | ATOM | 3241 | C   | GLU | A | 412 | 16.960 | 22.532 | 53.366 | 1.00 | 24.56  |
|    | ATOM | 3242 | O   | GLU | A | 412 | 16.045 | 22.612 | 52.555 | 1.00 | 26.86  |
|    | ATOM | 3243 | CB  | GLU | A | 412 | 19.330 | 22.211 | 52.913 | 1.00 | 28.91  |
|    | ATOM | 3244 | CG  | GLU | A | 412 | 20.206 | 22.405 | 51.660 | 1.00 | 51.34  |
|    | ATOM | 3245 | CD  | GLU | A | 412 | 21.671 | 22.089 | 51.908 | 1.00 | 100.00 |
| 60 | ATOM | 3246 | OE1 | GLU | A | 412 | 22.243 | 22.331 | 52.963 | 1.00 | 100.00 |
|    | ATOM | 3247 | OE2 | GLU | A | 412 | 22.274 | 21.541 | 50.874 | 1.00 | 100.00 |
|    | ATOM | 3248 | N   | LYS | A | 413 | 16.909 | 21.757 | 54.442 | 1.00 | 19.78  |
|    | ATOM | 3249 | CA  | LYS | A | 413 | 15.755 | 20.940 | 54.747 | 1.00 | 15.53  |
|    | ATOM | 3250 | C   | LYS | A | 413 | 14.484 | 21.718 | 54.892 | 1.00 | 22.00  |



|    |      |      |     |     |   |     |        |        |        |      |        |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
|    | ATOM | 3251 | O   | LYS | A | 413 | 13.464 | 21.272 | 54.409 | 1.00 | 23.41  |
|    | ATOM | 3252 | CB  | LYS | A | 413 | 16.020 | 20.156 | 56.008 | 1.00 | 17.04  |
|    | ATOM | 3253 | CG  | LYS | A | 413 | 14.754 | 19.602 | 56.629 | 1.00 | 26.97  |
| 5  | ATOM | 3254 | CD  | LYS | A | 413 | 14.225 | 18.351 | 55.955 | 1.00 | 37.17  |
|    | ATOM | 3255 | CE  | LYS | A | 413 | 13.553 | 17.352 | 56.893 | 1.00 | 56.50  |
|    | ATOM | 3256 | NZ  | LYS | A | 413 | 13.126 | 16.109 | 56.223 | 1.00 | 80.78  |
|    | ATOM | 3257 | N   | PHE | A | 414 | 14.543 | 22.888 | 55.532 | 1.00 | 19.76  |
|    | ATOM | 3258 | CA  | PHE | A | 414 | 13.366 | 23.700 | 55.808 | 1.00 | 17.00  |
| 10 | ATOM | 3259 | C   | PHE | A | 414 | 13.192 | 24.945 | 54.985 | 1.00 | 21.55  |
|    | ATOM | 3260 | O   | PHE | A | 414 | 12.329 | 25.748 | 55.303 | 1.00 | 17.11  |
|    | ATOM | 3261 | CB  | PHE | A | 414 | 13.219 | 24.035 | 57.303 | 1.00 | 16.42  |
|    | ATOM | 3262 | CG  | PHE | A | 414 | 13.047 | 22.800 | 58.122 | 1.00 | 15.55  |
|    | ATOM | 3263 | CD1 | PHE | A | 414 | 11.894 | 22.029 | 57.979 | 1.00 | 19.53  |
|    | ATOM | 3264 | CD2 | PHE | A | 414 | 14.024 | 22.368 | 59.015 | 1.00 | 20.06  |
| 15 | ATOM | 3265 | CE1 | PHE | A | 414 | 11.709 | 20.868 | 58.729 | 1.00 | 18.22  |
|    | ATOM | 3266 | CE2 | PHE | A | 414 | 13.861 | 21.205 | 59.771 | 1.00 | 21.10  |
|    | ATOM | 3267 | CZ  | PHE | A | 414 | 12.695 | 20.456 | 59.627 | 1.00 | 19.80  |
|    | ATOM | 3268 | N   | SER | A | 415 | 13.972 | 25.111 | 53.928 | 1.00 | 22.05  |
| 20 | ATOM | 3269 | CA  | SER | A | 415 | 13.807 | 26.273 | 53.044 | 1.00 | 23.12  |
|    | ATOM | 3270 | C   | SER | A | 415 | 12.380 | 26.434 | 52.548 | 1.00 | 23.50  |
|    | ATOM | 3271 | O   | SER | A | 415 | 11.775 | 25.451 | 52.138 | 1.00 | 22.71  |
|    | ATOM | 3272 | CB  | SER | A | 415 | 14.763 | 26.214 | 51.858 | 1.00 | 23.04  |
|    | ATOM | 3273 | OG  | SER | A | 415 | 16.054 | 26.591 | 52.319 | 1.00 | 31.15  |
| 25 | ATOM | 3274 | N   | TYR | A | 416 | 11.860 | 27.670 | 52.600 | 1.00 | 21.68  |
|    | ATOM | 3275 | CA  | TYR | A | 416 | 10.506 | 28.036 | 52.165 | 1.00 | 22.03  |
|    | ATOM | 3276 | C   | TYR | A | 416 | 9.401  | 27.514 | 53.056 | 1.00 | 22.90  |
|    | ATOM | 3277 | O   | TYR | A | 416 | 8.239  | 27.556 | 52.681 | 1.00 | 19.44  |
|    | ATOM | 3278 | CB  | TYR | A | 416 | 10.181 | 27.732 | 50.669 | 1.00 | 21.41  |
| 30 | ATOM | 3279 | CG  | TYR | A | 416 | 11.390 | 28.011 | 49.812 | 1.00 | 21.01  |
|    | ATOM | 3280 | CD1 | TYR | A | 416 | 12.232 | 27.003 | 49.339 | 1.00 | 22.57  |
|    | ATOM | 3281 | CD2 | TYR | A | 416 | 11.686 | 29.339 | 49.509 | 1.00 | 20.93  |
|    | ATOM | 3282 | CE1 | TYR | A | 416 | 13.354 | 27.305 | 48.566 | 1.00 | 19.33  |
|    | ATOM | 3283 | CE2 | TYR | A | 416 | 12.792 | 29.665 | 48.729 | 1.00 | 23.16  |
| 35 | ATOM | 3284 | CZ  | TYR | A | 416 | 13.628 | 28.643 | 48.271 | 1.00 | 32.30  |
|    | ATOM | 3285 | OH  | TYR | A | 416 | 14.715 | 28.959 | 47.491 | 1.00 | 25.33  |
|    | ATOM | 3286 | N   | LYS | A | 417 | 9.747  | 27.012 | 54.230 | 1.00 | 21.98  |
|    | ATOM | 3287 | CA  | LYS | A | 417 | 8.749  | 26.482 | 55.127 | 1.00 | 20.82  |
|    | ATOM | 3288 | C   | LYS | A | 417 | 8.702  | 27.284 | 56.408 | 1.00 | 20.61  |
| 40 | ATOM | 3289 | O   | LYS | A | 417 | 9.629  | 28.038 | 56.671 | 1.00 | 18.79  |
|    | ATOM | 3290 | CB  | LYS | A | 417 | 9.115  | 25.041 | 55.481 | 1.00 | 22.26  |
|    | ATOM | 3291 | CG  | LYS | A | 417 | 9.094  | 24.078 | 54.266 | 1.00 | 29.52  |
|    | ATOM | 3292 | CD  | LYS | A | 417 | 7.999  | 24.355 | 53.237 | 1.00 | 72.37  |
|    | ATOM | 3293 | CE  | LYS | A | 417 | 8.204  | 23.679 | 51.876 | 1.00 | 100.00 |
| 45 | ATOM | 3294 | NZ  | LYS | A | 417 | 7.124  | 23.931 | 50.895 | 1.00 | 100.00 |
|    | ATOM | 3295 | N   | SER | A | 418 | 7.645  | 27.068 | 57.177 | 1.00 | 17.88  |
|    | ATOM | 3296 | CA  | SER | A | 418 | 7.429  | 27.702 | 58.478 | 1.00 | 19.91  |
|    | ATOM | 3297 | C   | SER | A | 418 | 7.410  | 26.538 | 59.459 | 1.00 | 23.93  |
|    | ATOM | 3298 | O   | SER | A | 418 | 6.660  | 25.601 | 59.227 | 1.00 | 21.09  |
| 50 | ATOM | 3299 | CB  | SER | A | 418 | 6.139  | 28.495 | 58.451 | 1.00 | 12.45  |
|    | ATOM | 3300 | OG  | SER | A | 418 | 6.279  | 29.520 | 57.494 | 1.00 | 17.15  |
|    | ATOM | 3301 | N   | ILE | A | 419 | 8.240  | 26.529 | 60.516 | 1.00 | 14.38  |
|    | ATOM | 3302 | CA  | ILE | A | 419 | 8.323  | 25.353 | 61.382 | 1.00 | 12.23  |
|    | ATOM | 3303 | C   | ILE | A | 419 | 8.330  | 25.695 | 62.841 | 1.00 | 16.49  |
| 55 | ATOM | 3304 | O   | ILE | A | 419 | 8.334  | 26.875 | 63.219 | 1.00 | 14.48  |
|    | ATOM | 3305 | CB  | ILE | A | 419 | 9.662  | 24.641 | 61.097 | 1.00 | 18.50  |
|    | ATOM | 3306 | CG1 | ILE | A | 419 | 10.782 | 25.649 | 61.392 | 1.00 | 18.34  |
|    | ATOM | 3307 | CG2 | ILE | A | 419 | 9.782  | 24.271 | 59.611 | 1.00 | 14.45  |
|    | ATOM | 3308 | CD1 | ILE | A | 419 | 12.163 | 25.028 | 61.473 | 1.00 | 22.79  |
| 60 | ATOM | 3309 | N   | THR | A | 420 | 8.320  | 24.635 | 63.644 | 1.00 | 16.31  |
|    | ATOM | 3310 | CA  | THR | A | 420 | 8.281  | 24.810 | 65.083 | 1.00 | 14.71  |
|    | ATOM | 3311 | C   | THR | A | 420 | 9.545  | 24.290 | 65.714 | 1.00 | 16.25  |
|    | ATOM | 3312 | O   | THR | A | 420 | 10.346 | 23.636 | 65.077 | 1.00 | 17.31  |
|    | ATOM | 3313 | CB  | THR | A | 420 | 7.118  | 24.004 | 65.697 | 1.00 | 17.59  |
|    | ATOM | 3314 | OG1 | THR | A | 420 | 7.437  | 22.645 | 65.519 | 1.00 | 17.59  |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
|    | ATOM | 3315 | CG2 | THR | A | 420 | 5.794  | 24.260 | 65.010 | 1.00 | 16.45 |
|    | ATOM | 3316 | N   | THR | A | 421 | 9.679  | 24.540 | 67.010 | 1.00 | 15.19 |
|    | ATOM | 3317 | CA  | THR | A | 421 | 10.782 | 24.047 | 67.818 | 1.00 | 15.49 |
| 5  | ATOM | 3318 | C   | THR | A | 421 | 10.930 | 22.520 | 67.618 | 1.00 | 21.17 |
|    | ATOM | 3319 | O   | THR | A | 421 | 12.041 | 22.044 | 67.401 | 1.00 | 18.91 |
|    | ATOM | 3320 | CB  | THR | A | 421 | 10.564 | 24.437 | 69.309 | 1.00 | 10.87 |
|    | ATOM | 3321 | OG1 | THR | A | 421 | 10.618 | 25.851 | 69.383 | 1.00 | 15.99 |
|    | ATOM | 3322 | CG2 | THR | A | 421 | 11.691 | 23.868 | 70.170 | 1.00 | 11.46 |
| 10 | ATOM | 3323 | N   | ASP | A | 422 | 9.829  | 21.736 | 67.673 | 1.00 | 18.70 |
|    | ATOM | 3324 | CA  | ASP | A | 422 | 9.885  | 20.262 | 67.467 | 1.00 | 16.03 |
|    | ATOM | 3325 | C   | ASP | A | 422 | 10.469 | 19.867 | 66.107 | 1.00 | 16.08 |
|    | ATOM | 3326 | O   | ASP | A | 422 | 11.273 | 18.932 | 65.958 | 1.00 | 16.68 |
|    | ATOM | 3327 | CB  | ASP | A | 422 | 8.523  | 19.568 | 67.581 | 1.00 | 16.64 |
| 15 | ATOM | 3328 | CG  | ASP | A | 422 | 8.719  | 18.079 | 67.574 | 1.00 | 26.85 |
|    | ATOM | 3329 | OD1 | ASP | A | 422 | 9.568  | 17.580 | 68.286 | 1.00 | 23.44 |
|    | ATOM | 3330 | OD2 | ASP | A | 422 | 7.924  | 17.366 | 66.787 | 1.00 | 23.32 |
|    | ATOM | 3331 | N   | ASP | A | 423 | 10.069 | 20.575 | 65.060 | 1.00 | 17.50 |
|    | ATOM | 3332 | CA  | ASP | A | 423 | 10.654 | 20.224 | 63.757 | 1.00 | 18.18 |
| 20 | ATOM | 3333 | C   | ASP | A | 423 | 12.148 | 20.442 | 63.826 | 1.00 | 17.70 |
|    | ATOM | 3334 | O   | ASP | A | 423 | 12.922 | 19.645 | 63.316 | 1.00 | 15.95 |
|    | ATOM | 3335 | CB  | ASP | A | 423 | 10.099 | 21.075 | 62.613 | 1.00 | 17.77 |
|    | ATOM | 3336 | CG  | ASP | A | 423 | 8.614  | 20.972 | 62.510 | 1.00 | 20.51 |
|    | ATOM | 3337 | OD1 | ASP | A | 423 | 8.042  | 19.936 | 62.718 | 1.00 | 29.77 |
| 25 | ATOM | 3338 | OD2 | ASP | A | 423 | 8.016  | 22.095 | 62.226 | 1.00 | 18.32 |
|    | ATOM | 3339 | N   | TRP | A | 424 | 12.559 | 21.545 | 64.459 | 1.00 | 12.60 |
|    | ATOM | 3340 | CA  | TRP | A | 424 | 13.979 | 21.793 | 64.555 | 1.00 | 14.79 |
|    | ATOM | 3341 | C   | TRP | A | 424 | 14.690 | 20.684 | 65.330 | 1.00 | 19.67 |
|    | ATOM | 3342 | O   | TRP | A | 424 | 15.731 | 20.154 | 64.939 | 1.00 | 16.84 |
| 30 | ATOM | 3343 | CB  | TRP | A | 424 | 14.187 | 23.134 | 65.283 | 1.00 | 14.84 |
|    | ATOM | 3344 | CG  | TRP | A | 424 | 15.603 | 23.332 | 65.711 | 1.00 | 13.71 |
|    | ATOM | 3345 | CD1 | TRP | A | 424 | 16.594 | 23.830 | 64.937 | 1.00 | 15.42 |
|    | ATOM | 3346 | CD2 | TRP | A | 424 | 16.185 | 23.060 | 67.002 | 1.00 | 13.68 |
|    | ATOM | 3347 | NE1 | TRP | A | 424 | 17.765 | 23.853 | 65.640 | 1.00 | 14.21 |
| 35 | ATOM | 3348 | CE2 | TRP | A | 424 | 17.558 | 23.383 | 66.909 | 1.00 | 13.75 |
|    | ATOM | 3349 | CE3 | TRP | A | 424 | 15.684 | 22.576 | 68.210 | 1.00 | 16.53 |
|    | ATOM | 3350 | CZ2 | TRP | A | 424 | 18.436 | 23.247 | 67.983 | 1.00 | 13.89 |
|    | ATOM | 3351 | CZ3 | TRP | A | 424 | 16.564 | 22.434 | 69.288 | 1.00 | 16.24 |
|    | ATOM | 3352 | CH2 | TRP | A | 424 | 17.919 | 22.786 | 69.175 | 1.00 | 15.55 |
| 40 | ATOM | 3353 | N   | LYS | A | 425 | 14.139 | 20.328 | 66.480 | 1.00 | 13.83 |
|    | ATOM | 3354 | CA  | LYS | A | 425 | 14.778 | 19.337 | 67.319 | 1.00 | 14.35 |
|    | ATOM | 3355 | C   | LYS | A | 425 | 14.705 | 17.914 | 66.753 | 1.00 | 19.43 |
|    | ATOM | 3356 | O   | LYS | A | 425 | 15.619 | 17.089 | 66.910 | 1.00 | 16.20 |
|    | ATOM | 3357 | CB  | LYS | A | 425 | 14.262 | 19.441 | 68.735 | 1.00 | 13.53 |
| 45 | ATOM | 3358 | CG  | LYS | A | 425 | 14.912 | 18.488 | 69.720 | 1.00 | 14.17 |
|    | ATOM | 3359 | CD  | LYS | A | 425 | 14.289 | 18.698 | 71.085 | 1.00 | 14.61 |
|    | ATOM | 3360 | CE  | LYS | A | 425 | 14.214 | 17.413 | 71.872 | 1.00 | 33.75 |
|    | ATOM | 3361 | NZ  | LYS | A | 425 | 12.961 | 16.707 | 71.574 | 1.00 | 28.69 |
|    | ATOM | 3362 | N   | ASP | A | 426 | 13.591 | 17.633 | 66.093 | 1.00 | 17.34 |
| 50 | ATOM | 3363 | CA  | ASP | A | 426 | 13.430 | 16.341 | 65.480 | 1.00 | 15.98 |
|    | ATOM | 3364 | C   | ASP | A | 426 | 14.524 | 16.256 | 64.383 | 1.00 | 23.28 |
|    | ATOM | 3365 | O   | ASP | A | 426 | 15.177 | 15.246 | 64.128 | 1.00 | 25.50 |
|    | ATOM | 3366 | CB  | ASP | A | 426 | 11.987 | 16.225 | 64.918 | 1.00 | 13.29 |
|    | ATOM | 3367 | CG  | ASP | A | 426 | 10.984 | 15.900 | 65.989 | 1.00 | 14.86 |
| 55 | ATOM | 3368 | OD1 | ASP | A | 426 | 11.296 | 15.712 | 67.147 | 1.00 | 19.08 |
|    | ATOM | 3369 | OD2 | ASP | A | 426 | 9.746  | 15.852 | 65.579 | 1.00 | 18.33 |
|    | ATOM | 3370 | N   | PHE | A | 427 | 14.770 | 17.354 | 63.684 | 1.00 | 20.60 |
|    | ATOM | 3371 | CA  | PHE | A | 427 | 15.789 | 17.331 | 62.633 | 1.00 | 20.61 |
|    | ATOM | 3372 | C   | PHE | A | 427 | 17.203 | 17.172 | 63.165 | 1.00 | 26.34 |
| 60 | ATOM | 3373 | O   | PHE | A | 427 | 18.056 | 16.476 | 62.592 | 1.00 | 22.98 |
|    | ATOM | 3374 | CB  | PHE | A | 427 | 15.712 | 18.535 | 61.679 | 1.00 | 20.77 |
|    | ATOM | 3375 | CG  | PHE | A | 427 | 16.772 | 18.432 | 60.611 | 1.00 | 24.06 |
|    | ATOM | 3376 | CD1 | PHE | A | 427 | 16.747 | 17.398 | 59.674 | 1.00 | 27.11 |
|    | ATOM | 3377 | CD2 | PHE | A | 427 | 17.815 | 19.355 | 60.549 | 1.00 | 24.52 |
|    | ATOM | 3378 | CE1 | PHE | A | 427 | 17.726 | 17.312 | 58.685 | 1.00 | 27.68 |



|    |      |      |     |     |   |     |        |        |        |      |        |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
|    | ATOM | 3379 | CE2 | PHE | A | 427 | 18.801 | 19.284 | 59.565 | 1.00 | 28.65  |
|    | ATOM | 3380 | CZ  | PHE | A | 427 | 18.756 | 18.254 | 58.629 | 1.00 | 24.74  |
|    | ATOM | 3381 | N   | LEU | A | 428 | 17.417 | 17.848 | 64.291 | 1.00 | 22.50  |
| 5  | ATOM | 3382 | CA  | LEU | A | 428 | 18.686 | 17.827 | 64.979 | 1.00 | 24.10  |
|    | ATOM | 3383 | C   | LEU | A | 428 | 19.053 | 16.391 | 65.339 | 1.00 | 22.01  |
|    | ATOM | 3384 | O   | LEU | A | 428 | 20.183 | 15.960 | 65.123 | 1.00 | 23.99  |
|    | ATOM | 3385 | CB  | LEU | A | 428 | 18.685 | 18.806 | 66.186 | 1.00 | 23.18  |
|    | ATOM | 3386 | CG  | LEU | A | 428 | 19.949 | 18.790 | 67.054 | 1.00 | 26.21  |
| 10 | ATOM | 3387 | CD1 | LEU | A | 428 | 21.120 | 19.538 | 66.421 | 1.00 | 25.09  |
|    | ATOM | 3388 | CD2 | LEU | A | 428 | 19.659 | 19.334 | 68.459 | 1.00 | 21.07  |
|    | ATOM | 3389 | N   | TYR | A | 429 | 18.087 | 15.650 | 65.866 | 1.00 | 16.35  |
|    | ATOM | 3390 | CA  | TYR | A | 429 | 18.278 | 14.259 | 66.241 | 1.00 | 15.82  |
|    | ATOM | 3391 | C   | TYR | A | 429 | 18.482 | 13.390 | 65.019 | 1.00 | 20.80  |
|    | ATOM | 3392 | O   | TYR | A | 429 | 19.216 | 12.416 | 64.997 | 1.00 | 21.02  |
| 15 | ATOM | 3393 | CB  | TYR | A | 429 | 17.037 | 13.759 | 66.940 | 1.00 | 14.93  |
|    | ATOM | 3394 | CG  | TYR | A | 429 | 17.232 | 13.841 | 68.426 | 1.00 | 19.52  |
|    | ATOM | 3395 | CD1 | TYR | A | 429 | 16.999 | 15.039 | 69.104 | 1.00 | 18.07  |
|    | ATOM | 3396 | CD2 | TYR | A | 429 | 17.667 | 12.710 | 69.121 | 1.00 | 17.20  |
| 20 | ATOM | 3397 | CE1 | TYR | A | 429 | 17.183 | 15.108 | 70.484 | 1.00 | 14.78  |
|    | ATOM | 3398 | CE2 | TYR | A | 429 | 17.850 | 12.752 | 70.496 | 1.00 | 15.85  |
|    | ATOM | 3399 | CZ  | TYR | A | 429 | 17.615 | 13.961 | 71.157 | 1.00 | 26.56  |
|    | ATOM | 3400 | OH  | TYR | A | 429 | 17.807 | 14.009 | 72.508 | 1.00 | 23.93  |
|    | ATOM | 3401 | N   | SER | A | 430 | 17.839 | 13.785 | 63.955 | 1.00 | 18.00  |
| 25 | ATOM | 3402 | CA  | SER | A | 430 | 17.986 | 13.048 | 62.735 | 1.00 | 20.34  |
|    | ATOM | 3403 | C   | SER | A | 430 | 19.392 | 13.282 | 62.136 | 1.00 | 28.86  |
|    | ATOM | 3404 | O   | SER | A | 430 | 20.133 | 12.347 | 61.797 | 1.00 | 25.84  |
|    | ATOM | 3405 | CB  | SER | A | 430 | 16.843 | 13.486 | 61.845 | 1.00 | 19.64  |
|    | ATOM | 3406 | OG  | SER | A | 430 | 16.960 | 12.766 | 60.657 | 1.00 | 32.88  |
| 30 | ATOM | 3407 | N   | TYR | A | 431 | 19.792 | 14.556 | 62.021 | 1.00 | 23.08  |
|    | ATOM | 3408 | CA  | TYR | A | 431 | 21.104 | 14.862 | 61.497 | 1.00 | 23.26  |
|    | ATOM | 3409 | C   | TYR | A | 431 | 22.209 | 14.166 | 62.288 | 1.00 | 31.19  |
|    | ATOM | 3410 | O   | TYR | A | 431 | 23.152 | 13.580 | 61.747 | 1.00 | 27.84  |
|    | ATOM | 3411 | CB  | TYR | A | 431 | 21.392 | 16.372 | 61.476 | 1.00 | 22.23  |
| 35 | ATOM | 3412 | CG  | TYR | A | 431 | 22.660 | 16.758 | 60.741 | 1.00 | 23.21  |
|    | ATOM | 3413 | CD1 | TYR | A | 431 | 22.665 | 16.994 | 59.365 | 1.00 | 26.21  |
|    | ATOM | 3414 | CD2 | TYR | A | 431 | 23.864 | 16.920 | 61.433 | 1.00 | 28.30  |
|    | ATOM | 3415 | CE1 | TYR | A | 431 | 23.836 | 17.354 | 58.692 | 1.00 | 33.33  |
|    | ATOM | 3416 | CE2 | TYR | A | 431 | 25.045 | 17.277 | 60.777 | 1.00 | 29.03  |
| 40 | ATOM | 3417 | CZ  | TYR | A | 431 | 25.032 | 17.498 | 59.401 | 1.00 | 33.73  |
|    | ATOM | 3418 | OH  | TYR | A | 431 | 26.201 | 17.881 | 58.802 | 1.00 | 30.59  |
|    | ATOM | 3419 | N   | PHE | A | 432 | 22.078 | 14.272 | 63.608 | 1.00 | 23.42  |
|    | ATOM | 3420 | CA  | PHE | A | 432 | 23.039 | 13.735 | 64.556 | 1.00 | 22.14  |
|    | ATOM | 3421 | C   | PHE | A | 432 | 22.659 | 12.334 | 65.001 | 1.00 | 27.48  |
| 45 | ATOM | 3422 | O   | PHE | A | 432 | 22.824 | 11.964 | 66.168 | 1.00 | 20.81  |
|    | ATOM | 3423 | CB  | PHE | A | 432 | 23.211 | 14.715 | 65.751 | 1.00 | 20.76  |
|    | ATOM | 3424 | CG  | PHE | A | 432 | 24.035 | 15.918 | 65.348 | 1.00 | 21.62  |
|    | ATOM | 3425 | CD1 | PHE | A | 432 | 25.364 | 15.674 | 65.025 | 1.00 | 25.75  |
|    | ATOM | 3426 | CD2 | PHE | A | 432 | 23.566 | 17.232 | 65.250 | 1.00 | 22.01  |
| 50 | ATOM | 3427 | CE1 | PHE | A | 432 | 26.202 | 16.708 | 64.619 | 1.00 | 26.06  |
|    | ATOM | 3428 | CE2 | PHE | A | 432 | 24.398 | 18.277 | 64.841 | 1.00 | 24.06  |
|    | ATOM | 3429 | CZ  | PHE | A | 432 | 25.732 | 18.014 | 64.539 | 1.00 | 22.97  |
|    | ATOM | 3430 | N   | LYS | A | 433 | 22.150 | 11.536 | 64.065 | 1.00 | 30.29  |
|    | ATOM | 3431 | CA  | LYS | A | 433 | 21.757 | 10.205 | 64.480 | 1.00 | 33.97  |
| 55 | ATOM | 3432 | C   | LYS | A | 433 | 22.886 | 9.408  | 65.113 | 1.00 | 40.77  |
|    | ATOM | 3433 | O   | LYS | A | 433 | 22.690 | 8.545  | 65.964 | 1.00 | 45.44  |
|    | ATOM | 3434 | CB  | LYS | A | 433 | 21.017 | 9.429  | 63.418 | 1.00 | 41.36  |
|    | ATOM | 3435 | CG  | LYS | A | 433 | 21.934 | 9.107  | 62.270 | 1.00 | 42.12  |
|    | ATOM | 3436 | CD  | LYS | A | 433 | 21.340 | 9.569  | 60.951 | 1.00 | 85.11  |
| 60 | ATOM | 3437 | CE  | LYS | A | 433 | 21.770 | 8.690  | 59.784 | 1.00 | 100.00 |
|    | ATOM | 3438 | NZ  | LYS | A | 433 | 21.052 | 8.990  | 58.530 | 1.00 | 100.00 |
|    | ATOM | 3439 | N   | ASP | A | 434 | 24.091 | 9.729  | 64.700 | 1.00 | 38.33  |
|    | ATOM | 3440 | CA  | ASP | A | 434 | 25.295 | 9.086  | 65.188 | 1.00 | 40.98  |
|    | ATOM | 3441 | C   | ASP | A | 434 | 25.640 | 9.549  | 66.594 | 1.00 | 42.43  |
|    | ATOM | 3442 | O   | ASP | A | 434 | 26.508 | 8.979  | 67.241 | 1.00 | 42.35  |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
|    | ATOM | 3443 | CB  | ASP | A | 434 | 26.493 | 9.429  | 64.250 | 1.00 | 47.81 |
|    | ATOM | 3444 | CG  | ASP | A | 434 | 26.762 | 10.919 | 64.034 | 1.00 | 73.28 |
|    | ATOM | 3445 | OD1 | ASP | A | 434 | 25.948 | 11.739 | 63.601 | 1.00 | 69.11 |
| 5  | ATOM | 3446 | OD2 | ASP | A | 434 | 28.007 | 11.242 | 64.314 | 1.00 | 80.38 |
|    | ATOM | 3447 | N   | LYS | A | 435 | 24.987 | 10.601 | 67.068 | 1.00 | 33.72 |
|    | ATOM | 3448 | CA  | LYS | A | 435 | 25.312 | 11.120 | 68.374 | 1.00 | 30.49 |
|    | ATOM | 3449 | C   | LYS | A | 435 | 24.122 | 11.247 | 69.306 | 1.00 | 32.57 |
|    | ATOM | 3450 | O   | LYS | A | 435 | 24.181 | 12.067 | 70.217 | 1.00 | 29.28 |
| 10 | ATOM | 3451 | CB  | LYS | A | 435 | 26.018 | 12.465 | 68.200 | 1.00 | 30.20 |
|    | ATOM | 3452 | CG  | LYS | A | 435 | 27.396 | 12.351 | 67.568 | 1.00 | 19.40 |
|    | ATOM | 3453 | CD  | LYS | A | 435 | 27.984 | 13.718 | 67.237 | 1.00 | 28.53 |
|    | ATOM | 3454 | CE  | LYS | A | 435 | 29.504 | 13.723 | 67.224 | 1.00 | 36.05 |
|    | ATOM | 3455 | NZ  | LYS | A | 435 | 30.078 | 14.696 | 66.281 | 1.00 | 38.07 |
| 15 | ATOM | 3456 | N   | VAL | A | 436 | 23.063 | 10.467 | 69.083 | 1.00 | 32.65 |
|    | ATOM | 3457 | CA  | VAL | A | 436 | 21.867 | 10.565 | 69.920 | 1.00 | 36.68 |
|    | ATOM | 3458 | C   | VAL | A | 436 | 22.189 | 10.528 | 71.391 | 1.00 | 39.39 |
|    | ATOM | 3459 | O   | VAL | A | 436 | 21.544 | 11.154 | 72.236 | 1.00 | 34.16 |
|    | ATOM | 3460 | CB  | VAL | A | 436 | 20.768 | 9.553  | 69.613 | 1.00 | 44.95 |
| 20 | ATOM | 3461 | CG1 | VAL | A | 436 | 20.016 | 9.971  | 68.355 | 1.00 | 45.77 |
|    | ATOM | 3462 | CG2 | VAL | A | 436 | 21.391 | 8.187  | 69.405 | 1.00 | 48.21 |
|    | ATOM | 3463 | N   | ASP | A | 437 | 23.205 | 9.740  | 71.670 | 1.00 | 40.66 |
|    | ATOM | 3464 | CA  | ASP | A | 437 | 23.663 | 9.569  | 73.019 | 1.00 | 39.64 |
|    | ATOM | 3465 | C   | ASP | A | 437 | 24.119 | 10.875 | 73.622 | 1.00 | 35.59 |
| 25 | ATOM | 3466 | O   | ASP | A | 437 | 23.871 | 11.128 | 74.785 | 1.00 | 36.38 |
|    | ATOM | 3467 | CB  | ASP | A | 437 | 24.686 | 8.437  | 73.136 | 1.00 | 42.27 |
|    | ATOM | 3468 | CG  | ASP | A | 437 | 23.976 | 7.123  | 73.303 | 1.00 | 64.05 |
|    | ATOM | 3469 | OD1 | ASP | A | 437 | 22.749 | 7.018  | 73.361 | 1.00 | 57.77 |
|    | ATOM | 3470 | OD2 | ASP | A | 437 | 24.825 | 6.121  | 73.385 | 1.00 | 89.95 |
| 30 | ATOM | 3471 | N   | VAL | A | 438 | 24.778 | 11.697 | 72.826 | 1.00 | 33.10 |
|    | ATOM | 3472 | CA  | VAL | A | 438 | 25.235 | 12.988 | 73.309 | 1.00 | 31.59 |
|    | ATOM | 3473 | C   | VAL | A | 438 | 24.012 | 13.879 | 73.521 | 1.00 | 28.65 |
|    | ATOM | 3474 | O   | VAL | A | 438 | 23.828 | 14.461 | 74.571 | 1.00 | 26.75 |
|    | ATOM | 3475 | CB  | VAL | A | 438 | 26.289 | 13.599 | 72.371 | 1.00 | 30.58 |
| 35 | ATOM | 3476 | CG1 | VAL | A | 438 | 26.809 | 14.928 | 72.920 | 1.00 | 27.87 |
|    | ATOM | 3477 | CG2 | VAL | A | 438 | 27.441 | 12.608 | 72.226 | 1.00 | 29.01 |
|    | ATOM | 3478 | N   | LEU | A | 439 | 23.179 | 13.926 | 72.494 | 1.00 | 22.69 |
|    | ATOM | 3479 | CA  | LEU | A | 439 | 21.952 | 14.698 | 72.466 | 1.00 | 20.02 |
|    | ATOM | 3480 | C   | LEU | A | 439 | 21.118 | 14.396 | 73.675 | 1.00 | 28.06 |
| 40 | ATOM | 3481 | O   | LEU | A | 439 | 20.547 | 15.279 | 74.289 | 1.00 | 31.30 |
|    | ATOM | 3482 | CB  | LEU | A | 439 | 21.125 | 14.403 | 71.201 | 1.00 | 17.24 |
|    | ATOM | 3483 | CG  | LEU | A | 439 | 21.769 | 15.002 | 69.960 | 1.00 | 19.41 |
|    | ATOM | 3484 | CD1 | LEU | A | 439 | 21.029 | 14.542 | 68.724 | 1.00 | 16.82 |
|    | ATOM | 3485 | CD2 | LEU | A | 439 | 21.748 | 16.528 | 70.034 | 1.00 | 23.96 |
| 45 | ATOM | 3486 | N   | ASN | A | 440 | 21.045 | 13.129 | 74.022 | 1.00 | 24.23 |
|    | ATOM | 3487 | CA  | ASN | A | 440 | 20.242 | 12.765 | 75.165 | 1.00 | 24.80 |
|    | ATOM | 3488 | C   | ASN | A | 440 | 20.785 | 13.294 | 76.473 | 1.00 | 29.26 |
|    | ATOM | 3489 | O   | ASN | A | 440 | 20.128 | 13.233 | 77.507 | 1.00 | 31.02 |
|    | ATOM | 3490 | CB  | ASN | A | 440 | 19.842 | 11.275 | 75.237 | 1.00 | 28.06 |
| 50 | ATOM | 3491 | CG  | ASN | A | 440 | 18.971 | 10.884 | 74.066 | 1.00 | 29.31 |
|    | ATOM | 3492 | OD1 | ASN | A | 440 | 19.138 | 9.820  | 73.451 | 1.00 | 40.12 |
|    | ATOM | 3493 | ND2 | ASN | A | 440 | 18.058 | 11.773 | 73.721 | 1.00 | 28.40 |
|    | ATOM | 3494 | N   | GLN | A | 441 | 21.984 | 13.833 | 76.434 | 1.00 | 26.30 |
|    | ATOM | 3495 | CA  | GLN | A | 441 | 22.535 | 14.361 | 77.656 | 1.00 | 27.26 |
| 55 | ATOM | 3496 | C   | GLN | A | 441 | 22.022 | 15.764 | 77.912 | 1.00 | 26.46 |
|    | ATOM | 3497 | O   | GLN | A | 441 | 22.203 | 16.336 | 78.988 | 1.00 | 25.27 |
|    | ATOM | 3498 | CB  | GLN | A | 441 | 24.073 | 14.404 | 77.609 | 1.00 | 32.14 |
|    | ATOM | 3499 | CG  | GLN | A | 441 | 24.762 | 13.016 | 77.641 | 1.00 | 49.60 |
|    | ATOM | 3500 | CD  | GLN | A | 441 | 26.057 | 13.019 | 76.850 | 1.00 | 66.63 |
| 60 | ATOM | 3501 | OE1 | GLN | A | 441 | 26.546 | 11.975 | 76.382 | 1.00 | 76.27 |
|    | ATOM | 3502 | NE2 | GLN | A | 441 | 26.608 | 14.217 | 76.676 | 1.00 | 56.68 |
|    | ATOM | 3503 | N   | VAL | A | 442 | 21.388 | 16.345 | 76.909 | 1.00 | 21.59 |
|    | ATOM | 3504 | CA  | VAL | A | 442 | 20.922 | 17.688 | 77.159 | 1.00 | 18.91 |
|    | ATOM | 3505 | C   | VAL | A | 442 | 19.615 | 17.729 | 77.897 | 1.00 | 19.52 |
|    | ATOM | 3506 | O   | VAL | A | 442 | 18.742 | 16.908 | 77.650 | 1.00 | 21.02 |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
|    | ATOM | 3507 | CB  | VAL | A | 442 | 20.898 | 18.538 | 75.917 | 1.00 | 19.77 |
|    | ATOM | 3508 | CG1 | VAL | A | 442 | 21.472 | 17.891 | 74.680 | 1.00 | 23.00 |
|    | ATOM | 3509 | CG2 | VAL | A | 442 | 19.787 | 19.580 | 75.787 | 1.00 | 13.26 |
| 5  | ATOM | 3510 | N   | ASP | A | 443 | 19.490 | 18.677 | 78.811 | 1.00 | 17.20 |
|    | ATOM | 3511 | CA  | ASP | A | 443 | 18.243 | 18.856 | 79.551 | 1.00 | 16.44 |
|    | ATOM | 3512 | C   | ASP | A | 443 | 17.277 | 19.752 | 78.727 | 1.00 | 17.64 |
|    | ATOM | 3513 | O   | ASP | A | 443 | 17.091 | 20.980 | 78.921 | 1.00 | 15.06 |
|    | ATOM | 3514 | CB  | ASP | A | 443 | 18.611 | 19.494 | 80.901 | 1.00 | 17.40 |
| 10 | ATOM | 3515 | CG  | ASP | A | 443 | 17.422 | 19.595 | 81.778 | 1.00 | 21.50 |
|    | ATOM | 3516 | OD1 | ASP | A | 443 | 16.309 | 19.286 | 81.395 | 1.00 | 26.57 |
|    | ATOM | 3517 | OD2 | ASP | A | 443 | 17.731 | 20.068 | 82.959 | 1.00 | 23.49 |
|    | ATOM | 3518 | N   | TRP | A | 444 | 16.675 | 19.105 | 77.736 | 1.00 | 15.54 |
|    | ATOM | 3519 | CA  | TRP | A | 444 | 15.763 | 19.759 | 76.816 | 1.00 | 16.92 |
| 15 | ATOM | 3520 | C   | TRP | A | 444 | 14.641 | 20.468 | 77.546 | 1.00 | 19.29 |
|    | ATOM | 3521 | O   | TRP | A | 444 | 14.292 | 21.572 | 77.194 | 1.00 | 18.00 |
|    | ATOM | 3522 | CB  | TRP | A | 444 | 15.195 | 18.747 | 75.793 | 1.00 | 13.71 |
|    | ATOM | 3523 | CG  | TRP | A | 444 | 16.267 | 18.226 | 74.892 | 1.00 | 14.88 |
|    | ATOM | 3524 | CD1 | TRP | A | 444 | 16.797 | 16.969 | 74.872 | 1.00 | 17.32 |
| 20 | ATOM | 3525 | CD2 | TRP | A | 444 | 16.952 | 18.958 | 73.861 | 1.00 | 16.34 |
|    | ATOM | 3526 | NE1 | TRP | A | 444 | 17.779 | 16.869 | 73.915 | 1.00 | 14.83 |
|    | ATOM | 3527 | CE2 | TRP | A | 444 | 17.880 | 18.063 | 73.255 | 1.00 | 16.96 |
|    | ATOM | 3528 | CE3 | TRP | A | 444 | 16.896 | 20.295 | 73.415 | 1.00 | 17.06 |
|    | ATOM | 3529 | CZ2 | TRP | A | 444 | 18.737 | 18.482 | 72.229 | 1.00 | 16.95 |
| 25 | ATOM | 3530 | CZ3 | TRP | A | 444 | 17.750 | 20.697 | 72.382 | 1.00 | 16.35 |
|    | ATOM | 3531 | CH2 | TRP | A | 444 | 18.664 | 19.807 | 71.806 | 1.00 | 16.47 |
|    | ATOM | 3532 | N   | ASN | A | 445 | 14.059 | 19.808 | 78.557 | 1.00 | 18.46 |
|    | ATOM | 3533 | CA  | ASN | A | 445 | 12.957 | 20.414 | 79.260 | 1.00 | 17.22 |
|    | ATOM | 3534 | C   | ASN | A | 445 | 13.334 | 21.761 | 79.837 | 1.00 | 20.45 |
| 30 | ATOM | 3535 | O   | ASN | A | 445 | 12.581 | 22.732 | 79.740 | 1.00 | 17.51 |
|    | ATOM | 3536 | CB  | ASN | A | 445 | 12.347 | 19.512 | 80.357 | 1.00 | 15.11 |
|    | ATOM | 3537 | CG  | ASN | A | 445 | 11.322 | 20.272 | 81.234 | 1.00 | 46.40 |
|    | ATOM | 3538 | OD1 | ASN | A | 445 | 11.526 | 20.515 | 82.448 | 1.00 | 39.99 |
|    | ATOM | 3539 | ND2 | ASN | A | 445 | 10.198 | 20.671 | 80.643 | 1.00 | 26.34 |
| 35 | ATOM | 3540 | N   | ALA | A | 446 | 14.504 | 21.791 | 80.484 | 1.00 | 18.70 |
|    | ATOM | 3541 | CA  | ALA | A | 446 | 14.918 | 23.022 | 81.091 | 1.00 | 16.75 |
|    | ATOM | 3542 | C   | ALA | A | 446 | 15.272 | 24.029 | 80.032 | 1.00 | 21.46 |
|    | ATOM | 3543 | O   | ALA | A | 446 | 14.765 | 25.172 | 80.030 | 1.00 | 20.55 |
|    | ATOM | 3544 | CB  | ALA | A | 446 | 16.049 | 22.774 | 82.055 | 1.00 | 19.42 |
| 40 | ATOM | 3545 | N   | TRP | A | 447 | 16.116 | 23.605 | 79.097 | 1.00 | 16.36 |
|    | ATOM | 3546 | CA  | TRP | A | 447 | 16.476 | 24.563 | 78.054 | 1.00 | 14.85 |
|    | ATOM | 3547 | C   | TRP | A | 447 | 15.277 | 25.163 | 77.279 | 1.00 | 18.68 |
|    | ATOM | 3548 | O   | TRP | A | 447 | 15.246 | 26.365 | 76.985 | 1.00 | 14.03 |
|    | ATOM | 3549 | CB  | TRP | A | 447 | 17.473 | 23.938 | 77.040 | 1.00 | 17.25 |
| 45 | ATOM | 3550 | CG  | TRP | A | 447 | 18.952 | 23.982 | 77.391 | 1.00 | 19.35 |
|    | ATOM | 3551 | CD1 | TRP | A | 447 | 19.697 | 22.957 | 77.930 | 1.00 | 22.25 |
|    | ATOM | 3552 | CD2 | TRP | A | 447 | 19.864 | 25.090 | 77.224 | 1.00 | 16.70 |
|    | ATOM | 3553 | NE1 | TRP | A | 447 | 21.007 | 23.356 | 78.105 | 1.00 | 19.46 |
|    | ATOM | 3554 | CE2 | TRP | A | 447 | 21.131 | 24.662 | 77.679 | 1.00 | 18.42 |
| 50 | ATOM | 3555 | CE3 | TRP | A | 447 | 19.737 | 26.403 | 76.766 | 1.00 | 16.34 |
|    | ATOM | 3556 | CZ2 | TRP | A | 447 | 22.241 | 25.512 | 77.625 | 1.00 | 16.76 |
|    | ATOM | 3557 | CZ3 | TRP | A | 447 | 20.854 | 27.230 | 76.705 | 1.00 | 14.87 |
|    | ATOM | 3558 | CH2 | TRP | A | 447 | 22.090 | 26.786 | 77.141 | 1.00 | 14.22 |
|    | ATOM | 3559 | N   | LEU | A | 448 | 14.275 | 24.336 | 76.899 | 1.00 | 14.96 |
| 55 | ATOM | 3560 | CA  | LEU | A | 448 | 13.146 | 24.835 | 76.096 | 1.00 | 16.27 |
|    | ATOM | 3561 | C   | LEU | A | 448 | 11.995 | 25.464 | 76.877 | 1.00 | 17.91 |
|    | ATOM | 3562 | O   | LEU | A | 448 | 11.332 | 26.404 | 76.398 | 1.00 | 13.49 |
|    | ATOM | 3563 | CB  | LEU | A | 448 | 12.522 | 23.690 | 75.238 | 1.00 | 16.42 |
|    | ATOM | 3564 | CG  | LEU | A | 448 | 13.500 | 22.945 | 74.302 | 1.00 | 16.43 |
| 60 | ATOM | 3565 | CD1 | LEU | A | 448 | 12.845 | 21.795 | 73.536 | 1.00 | 15.65 |
|    | ATOM | 3566 | CD2 | LEU | A | 448 | 14.163 | 23.901 | 73.315 | 1.00 | 12.87 |
|    | ATOM | 3567 | N   | TYR | A | 449 | 11.733 | 24.874 | 78.048 | 1.00 | 15.32 |
|    | ATOM | 3568 | CA  | TYR | A | 449 | 10.557 | 25.255 | 78.826 | 1.00 | 15.36 |
|    | ATOM | 3569 | C   | TYR | A | 449 | 10.763 | 25.822 | 80.198 | 1.00 | 19.93 |
|    | ATOM | 3570 | O   | TYR | A | 449 | 9.763  | 26.226 | 80.806 | 1.00 | 21.29 |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
|    | ATOM | 3571 | CB  | TYR | A | 449 | 9.611  | 24.031 | 78.983 | 1.00 | 14.65 |
|    | ATOM | 3572 | CG  | TYR | A | 449 | 9.473  | 23.315 | 77.667 | 1.00 | 17.69 |
|    | ATOM | 3573 | CD1 | TYR | A | 449 | 9.117  | 24.048 | 76.533 | 1.00 | 22.12 |
| 5  | ATOM | 3574 | CD2 | TYR | A | 449 | 9.771  | 21.958 | 77.541 | 1.00 | 19.27 |
|    | ATOM | 3575 | CE1 | TYR | A | 449 | 9.010  | 23.432 | 75.286 | 1.00 | 21.15 |
|    | ATOM | 3576 | CE2 | TYR | A | 449 | 9.669  | 21.318 | 76.301 | 1.00 | 18.29 |
|    | ATOM | 3577 | CZ  | TYR | A | 449 | 9.301  | 22.070 | 75.183 | 1.00 | 25.71 |
|    | ATOM | 3578 | OH  | TYR | A | 449 | 9.216  | 21.480 | 73.951 | 1.00 | 26.15 |
| 10 | ATOM | 3579 | N   | SER | A | 450 | 11.985 | 25.806 | 80.724 | 1.00 | 15.79 |
|    | ATOM | 3580 | CA  | SER | A | 450 | 12.156 | 26.362 | 82.061 | 1.00 | 14.12 |
|    | ATOM | 3581 | C   | SER | A | 450 | 12.474 | 27.864 | 82.025 | 1.00 | 16.42 |
|    | ATOM | 3582 | O   | SER | A | 450 | 13.127 | 28.340 | 81.109 | 1.00 | 15.32 |
|    | ATOM | 3583 | CB  | SER | A | 450 | 13.136 | 25.567 | 82.938 | 1.00 | 20.04 |
|    | ATOM | 3584 | OG  | SER | A | 450 | 12.687 | 24.254 | 83.189 | 1.00 | 16.61 |
| 15 | ATOM | 3585 | N   | PRO | A | 451 | 11.995 | 28.645 | 83.014 | 1.00 | 14.16 |
|    | ATOM | 3586 | CA  | PRO | A | 451 | 12.287 | 30.052 | 83.032 | 1.00 | 12.96 |
|    | ATOM | 3587 | C   | PRO | A | 451 | 13.696 | 30.228 | 83.581 | 1.00 | 15.11 |
|    | ATOM | 3588 | O   | PRO | A | 451 | 14.347 | 29.259 | 83.997 | 1.00 | 15.64 |
| 20 | ATOM | 3589 | CB  | PRO | A | 451 | 11.274 | 30.669 | 84.029 | 1.00 | 11.76 |
|    | ATOM | 3590 | CG  | PRO | A | 451 | 10.903 | 29.560 | 84.988 | 1.00 | 16.01 |
|    | ATOM | 3591 | CD  | PRO | A | 451 | 11.298 | 28.259 | 84.288 | 1.00 | 15.25 |
|    | ATOM | 3592 | N   | GLY | A | 452 | 14.148 | 31.481 | 83.586 | 1.00 | 12.85 |
|    | ATOM | 3593 | CA  | GLY | A | 452 | 15.430 | 31.822 | 84.160 | 1.00 | 12.46 |
| 25 | ATOM | 3594 | C   | GLY | A | 452 | 16.652 | 31.517 | 83.311 | 1.00 | 17.53 |
|    | ATOM | 3595 | O   | GLY | A | 452 | 16.559 | 31.320 | 82.117 | 1.00 | 14.38 |
|    | ATOM | 3596 | N   | LEU | A | 453 | 17.839 | 31.539 | 83.926 | 1.00 | 17.18 |
|    | ATOM | 3597 | CA  | LEU | A | 453 | 19.054 | 31.268 | 83.196 | 1.00 | 14.53 |
|    | ATOM | 3598 | C   | LEU | A | 453 | 19.087 | 29.819 | 82.762 | 1.00 | 14.71 |
| 30 | ATOM | 3599 | O   | LEU | A | 453 | 18.523 | 28.978 | 83.456 | 1.00 | 16.06 |
|    | ATOM | 3600 | CB  | LEU | A | 453 | 20.296 | 31.588 | 84.031 | 1.00 | 14.09 |
|    | ATOM | 3601 | CG  | LEU | A | 453 | 20.526 | 33.091 | 84.216 | 1.00 | 18.81 |
|    | ATOM | 3602 | CD1 | LEU | A | 453 | 21.635 | 33.253 | 85.247 | 1.00 | 16.98 |
|    | ATOM | 3603 | CD2 | LEU | A | 453 | 21.001 | 33.761 | 82.919 | 1.00 | 21.45 |
| 35 | ATOM | 3604 | N   | PRO | A | 454 | 19.770 | 29.537 | 81.637 | 1.00 | 15.62 |
|    | ATOM | 3605 | CA  | PRO | A | 454 | 19.907 | 28.194 | 81.119 | 1.00 | 15.68 |
|    | ATOM | 3606 | C   | PRO | A | 454 | 20.486 | 27.258 | 82.170 | 1.00 | 21.35 |
|    | ATOM | 3607 | O   | PRO | A | 454 | 21.236 | 27.662 | 83.039 | 1.00 | 21.73 |
|    | ATOM | 3608 | CB  | PRO | A | 454 | 20.918 | 28.317 | 79.965 | 1.00 | 16.56 |
| 40 | ATOM | 3609 | CG  | PRO | A | 454 | 20.906 | 29.751 | 79.501 | 1.00 | 16.74 |
|    | ATOM | 3610 | CD  | PRO | A | 454 | 20.290 | 30.524 | 80.640 | 1.00 | 15.71 |
|    | ATOM | 3611 | N   | PRO | A | 455 | 20.146 | 25.978 | 82.079 | 1.00 | 16.53 |
|    | ATOM | 3612 | CA  | PRO | A | 455 | 20.619 | 24.976 | 83.005 | 1.00 | 16.33 |
|    | ATOM | 3613 | C   | PRO | A | 455 | 22.146 | 24.834 | 83.016 | 1.00 | 25.51 |
| 45 | ATOM | 3614 | O   | PRO | A | 455 | 22.718 | 24.370 | 83.999 | 1.00 | 24.17 |
|    | ATOM | 3615 | CB  | PRO | A | 455 | 19.999 | 23.666 | 82.520 | 1.00 | 17.40 |
|    | ATOM | 3616 | CG  | PRO | A | 455 | 19.523 | 23.888 | 81.094 | 1.00 | 21.81 |
|    | ATOM | 3617 | CD  | PRO | A | 455 | 19.403 | 25.389 | 80.932 | 1.00 | 19.90 |
|    | ATOM | 3618 | N   | ILE | A | 456 | 22.816 | 25.205 | 81.916 | 1.00 | 20.88 |
| 50 | ATOM | 3619 | CA  | ILE | A | 456 | 24.262 | 25.117 | 81.810 | 1.00 | 17.40 |
|    | ATOM | 3620 | C   | ILE | A | 456 | 24.822 | 26.292 | 81.000 | 1.00 | 19.27 |
|    | ATOM | 3621 | O   | ILE | A | 456 | 24.191 | 26.798 | 80.064 | 1.00 | 17.96 |
|    | ATOM | 3622 | CB  | ILE | A | 456 | 24.675 | 23.737 | 81.316 | 1.00 | 23.45 |
|    | ATOM | 3623 | CG1 | ILE | A | 456 | 26.173 | 23.543 | 81.456 | 1.00 | 27.66 |
|    | ATOM | 3624 | CG2 | ILE | A | 456 | 24.285 | 23.529 | 79.865 | 1.00 | 26.37 |
| 55 | ATOM | 3625 | CD1 | ILE | A | 456 | 26.571 | 22.167 | 80.951 | 1.00 | 35.97 |
|    | ATOM | 3626 | N   | LYS | A | 457 | 26.011 | 26.772 | 81.383 | 1.00 | 15.81 |
|    | ATOM | 3627 | CA  | LYS | A | 457 | 26.649 | 27.883 | 80.697 | 1.00 | 17.12 |
|    | ATOM | 3628 | C   | LYS | A | 457 | 27.727 | 27.333 | 79.815 | 1.00 | 18.91 |
|    | ATOM | 3629 | O   | LYS | A | 457 | 28.541 | 26.562 | 80.281 | 1.00 | 17.84 |
| 60 | ATOM | 3630 | CB  | LYS | A | 457 | 27.308 | 28.793 | 81.727 | 1.00 | 16.24 |
|    | ATOM | 3631 | CG  | LYS | A | 457 | 27.896 | 30.067 | 81.130 | 1.00 | 16.93 |
|    | ATOM | 3632 | CD  | LYS | A | 457 | 28.245 | 31.062 | 82.227 | 1.00 | 10.77 |
|    | ATOM | 3633 | CE  | LYS | A | 457 | 28.785 | 32.347 | 81.659 | 1.00 | 11.49 |
|    | ATOM | 3634 | NZ  | LYS | A | 457 | 29.467 | 33.164 | 82.683 | 1.00 | 18.20 |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
|    | ATOM | 3635 | N   | PRO | A | 458 | 27.733 | 27.708 | 78.558 | 1.00 | 15.31 |
|    | ATOM | 3636 | CA  | PRO | A | 458 | 28.780 | 27.205 | 77.655 | 1.00 | 13.94 |
|    | ATOM | 3637 | C   | PRO | A | 458 | 30.169 | 27.681 | 78.096 | 1.00 | 16.97 |
| 5  | ATOM | 3638 | O   | PRO | A | 458 | 30.341 | 28.456 | 79.036 | 1.00 | 14.39 |
|    | ATOM | 3639 | CB  | PRO | A | 458 | 28.465 | 27.835 | 76.274 | 1.00 | 13.66 |
|    | ATOM | 3640 | CG  | PRO | A | 458 | 27.036 | 28.364 | 76.363 | 1.00 | 14.88 |
|    | ATOM | 3641 | CD  | PRO | A | 458 | 26.702 | 28.535 | 77.855 | 1.00 | 10.08 |
|    | ATOM | 3642 | N   | ASN | A | 459 | 31.199 | 27.223 | 77.408 | 1.00 | 17.07 |
| 10 | ATOM | 3643 | CA  | ASN | A | 459 | 32.546 | 27.672 | 77.722 | 1.00 | 15.61 |
|    | ATOM | 3644 | C   | ASN | A | 459 | 32.924 | 28.839 | 76.793 | 1.00 | 22.19 |
|    | ATOM | 3645 | O   | ASN | A | 459 | 32.647 | 28.812 | 75.578 | 1.00 | 20.83 |
|    | ATOM | 3646 | CB  | ASN | A | 459 | 33.580 | 26.559 | 77.455 | 1.00 | 19.60 |
|    | ATOM | 3647 | CG  | ASN | A | 459 | 33.158 | 25.288 | 78.136 | 1.00 | 26.10 |
| 15 | ATOM | 3648 | OD1 | ASN | A | 459 | 32.952 | 25.278 | 79.347 | 1.00 | 25.15 |
|    | ATOM | 3649 | ND2 | ASN | A | 459 | 32.972 | 24.236 | 77.361 | 1.00 | 24.39 |
|    | ATOM | 3650 | N   | TYR | A | 460 | 33.620 | 29.849 | 77.341 | 1.00 | 13.51 |
|    | ATOM | 3651 | CA  | TYR | A | 460 | 34.021 | 30.994 | 76.536 | 1.00 | 14.52 |
|    | ATOM | 3652 | C   | TYR | A | 460 | 35.485 | 31.370 | 76.683 | 1.00 | 16.97 |
| 20 | ATOM | 3653 | O   | TYR | A | 460 | 36.003 | 31.442 | 77.802 | 1.00 | 13.34 |
|    | ATOM | 3654 | CB  | TYR | A | 460 | 33.266 | 32.254 | 76.990 | 1.00 | 12.53 |
|    | ATOM | 3655 | CG  | TYR | A | 460 | 31.764 | 32.129 | 76.980 | 1.00 | 13.07 |
|    | ATOM | 3656 | CD1 | TYR | A | 460 | 31.070 | 31.553 | 78.046 | 1.00 | 17.79 |
|    | ATOM | 3657 | CD2 | TYR | A | 460 | 31.043 | 32.584 | 75.880 | 1.00 | 12.08 |
| 25 | ATOM | 3658 | CE1 | TYR | A | 460 | 29.677 | 31.450 | 78.049 | 1.00 | 16.54 |
|    | ATOM | 3659 | CE2 | TYR | A | 460 | 29.654 | 32.477 | 75.861 | 1.00 | 11.82 |
|    | ATOM | 3660 | CZ  | TYR | A | 460 | 28.971 | 31.911 | 76.938 | 1.00 | 16.71 |
|    | ATOM | 3661 | OH  | TYR | A | 460 | 27.589 | 31.834 | 76.894 | 1.00 | 15.52 |
|    | ATOM | 3662 | N   | ASP | A | 461 | 36.098 | 31.706 | 75.558 | 1.00 | 13.99 |
| 30 | ATOM | 3663 | CA  | ASP | A | 461 | 37.463 | 32.218 | 75.579 | 1.00 | 13.74 |
|    | ATOM | 3664 | C   | ASP | A | 461 | 37.414 | 33.608 | 76.255 | 1.00 | 16.51 |
|    | ATOM | 3665 | O   | ASP | A | 461 | 36.516 | 34.415 | 75.966 | 1.00 | 15.04 |
|    | ATOM | 3666 | CB  | ASP | A | 461 | 37.968 | 32.336 | 74.133 | 1.00 | 12.98 |
|    | ATOM | 3667 | CG  | ASP | A | 461 | 39.393 | 32.801 | 74.148 | 1.00 | 25.31 |
| 35 | ATOM | 3668 | OD1 | ASP | A | 461 | 40.335 | 32.064 | 74.314 | 1.00 | 40.40 |
|    | ATOM | 3669 | OD2 | ASP | A | 461 | 39.520 | 34.087 | 74.051 | 1.00 | 19.41 |
|    | ATOM | 3670 | N   | MET | A | 462 | 38.339 | 33.887 | 77.191 | 1.00 | 12.14 |
|    | ATOM | 3671 | CA  | MET | A | 462 | 38.359 | 35.144 | 77.928 | 1.00 | 9.92  |
|    | ATOM | 3672 | C   | MET | A | 462 | 39.312 | 36.203 | 77.406 | 1.00 | 15.43 |
| 40 | ATOM | 3673 | O   | MET | A | 462 | 39.413 | 37.265 | 77.958 | 1.00 | 15.61 |
|    | ATOM | 3674 | CB  | MET | A | 462 | 38.688 | 34.910 | 79.404 | 1.00 | 9.27  |
|    | ATOM | 3675 | CG  | MET | A | 462 | 37.716 | 33.909 | 79.977 | 1.00 | 13.43 |
|    | ATOM | 3676 | SD  | MET | A | 462 | 36.053 | 34.635 | 80.074 | 1.00 | 19.12 |
|    | ATOM | 3677 | CE  | MET | A | 462 | 36.505 | 35.919 | 81.264 | 1.00 | 17.88 |
| 45 | ATOM | 3678 | N   | THR | A | 463 | 40.037 | 35.922 | 76.347 | 1.00 | 13.87 |
|    | ATOM | 3679 | CA  | THR | A | 463 | 41.004 | 36.860 | 75.849 | 1.00 | 12.21 |
|    | ATOM | 3680 | C   | THR | A | 463 | 40.675 | 38.339 | 75.910 | 1.00 | 16.34 |
|    | ATOM | 3681 | O   | THR | A | 463 | 41.365 | 39.106 | 76.567 | 1.00 | 16.05 |
|    | ATOM | 3682 | CB  | THR | A | 463 | 41.595 | 36.434 | 74.489 | 1.00 | 17.83 |
| 50 | ATOM | 3683 | OG1 | THR | A | 463 | 41.940 | 35.051 | 74.538 | 1.00 | 14.22 |
|    | ATOM | 3684 | CG2 | THR | A | 463 | 42.841 | 37.298 | 74.204 | 1.00 | 15.70 |
|    | ATOM | 3685 | N   | LEU | A | 464 | 39.679 | 38.762 | 75.136 | 1.00 | 14.21 |
|    | ATOM | 3686 | CA  | LEU | A | 464 | 39.262 | 40.154 | 75.060 | 1.00 | 13.52 |
|    | ATOM | 3687 | C   | LEU | A | 464 | 38.408 | 40.679 | 76.228 | 1.00 | 12.70 |
| 55 | ATOM | 3688 | O   | LEU | A | 464 | 38.259 | 41.881 | 76.442 | 1.00 | 15.39 |
|    | ATOM | 3689 | CB  | LEU | A | 464 | 38.508 | 40.348 | 73.725 | 1.00 | 13.87 |
|    | ATOM | 3690 | CG  | LEU | A | 464 | 39.363 | 40.009 | 72.495 | 1.00 | 18.04 |
|    | ATOM | 3691 | CD1 | LEU | A | 464 | 38.448 | 40.076 | 71.260 | 1.00 | 14.36 |
|    | ATOM | 3692 | CD2 | LEU | A | 464 | 40.490 | 41.054 | 72.345 | 1.00 | 17.86 |
| 60 | ATOM | 3693 | N   | THR | A | 465 | 37.808 | 39.770 | 76.979 | 1.00 | 11.81 |
|    | ATOM | 3694 | CA  | THR | A | 465 | 36.946 | 40.116 | 78.103 | 1.00 | 10.62 |
|    | ATOM | 3695 | C   | THR | A | 465 | 37.728 | 40.487 | 79.360 | 1.00 | 17.70 |
|    | ATOM | 3696 | O   | THR | A | 465 | 37.361 | 41.359 | 80.131 | 1.00 | 15.35 |
|    | ATOM | 3697 | CB  | THR | A | 465 | 35.996 | 38.934 | 78.368 | 1.00 | 12.56 |
|    | ATOM | 3698 | OG1 | THR | A | 465 | 35.209 | 38.765 | 77.199 | 1.00 | 16.68 |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
|    | ATOM | 3699 | CG2 | THR | A | 465 | 35.075 | 39.241 | 79.545 | 1.00 | 17.17 |
|    | ATOM | 3700 | N   | ASN | A | 466 | 38.828 | 39.785 | 79.584 | 1.00 | 14.17 |
|    | ATOM | 3701 | CA  | ASN | A | 466 | 39.639 | 40.017 | 80.738 | 1.00 | 14.86 |
| 5  | ATOM | 3702 | C   | ASN | A | 466 | 39.933 | 41.491 | 81.017 | 1.00 | 16.02 |
|    | ATOM | 3703 | O   | ASN | A | 466 | 39.843 | 41.892 | 82.177 | 1.00 | 17.05 |
|    | ATOM | 3704 | CB  | ASN | A | 466 | 40.942 | 39.197 | 80.694 | 1.00 | 14.48 |
|    | ATOM | 3705 | CG  | ASN | A | 466 | 40.787 | 37.705 | 80.932 | 1.00 | 22.10 |
|    | ATOM | 3706 | OD1 | ASN | A | 466 | 41.539 | 36.878 | 80.386 | 1.00 | 21.72 |
| 10 | ATOM | 3707 | ND2 | ASN | A | 466 | 39.925 | 37.356 | 81.852 | 1.00 | 11.12 |
|    | ATOM | 3708 | N   | ALA | A | 467 | 40.313 | 42.307 | 80.012 | 1.00 | 16.17 |
|    | ATOM | 3709 | CA  | ALA | A | 467 | 40.614 | 43.704 | 80.336 | 1.00 | 16.10 |
|    | ATOM | 3710 | C   | ALA | A | 467 | 39.394 | 44.448 | 80.871 | 1.00 | 20.19 |
|    | ATOM | 3711 | O   | ALA | A | 467 | 39.488 | 45.363 | 81.722 | 1.00 | 17.63 |
| 15 | ATOM | 3712 | CB  | ALA | A | 467 | 41.159 | 44.411 | 79.118 | 1.00 | 14.71 |
|    | ATOM | 3713 | N   | CYS | A | 468 | 38.227 | 44.022 | 80.343 | 1.00 | 15.87 |
|    | ATOM | 3714 | CA  | CYS | A | 468 | 36.938 | 44.608 | 80.712 | 1.00 | 13.86 |
|    | ATOM | 3715 | C   | CYS | A | 468 | 36.609 | 44.369 | 82.167 | 1.00 | 15.16 |
|    | ATOM | 3716 | O   | CYS | A | 468 | 36.229 | 45.234 | 82.931 | 1.00 | 17.79 |
| 20 | ATOM | 3717 | CB  | CYS | A | 468 | 35.820 | 44.045 | 79.808 | 1.00 | 11.73 |
|    | ATOM | 3718 | SG  | CYS | A | 468 | 36.215 | 44.458 | 78.102 | 1.00 | 15.87 |
|    | ATOM | 3719 | N   | ILE | A | 469 | 36.811 | 43.145 | 82.571 | 1.00 | 13.83 |
|    | ATOM | 3720 | CA  | ILE | A | 469 | 36.531 | 42.747 | 83.941 | 1.00 | 11.80 |
|    | ATOM | 3721 | C   | ILE | A | 469 | 37.488 | 43.393 | 84.910 | 1.00 | 16.06 |
| 25 | ATOM | 3722 | O   | ILE | A | 469 | 37.076 | 43.848 | 85.970 | 1.00 | 18.22 |
|    | ATOM | 3723 | CB  | ILE | A | 469 | 36.659 | 41.230 | 84.042 | 1.00 | 15.30 |
|    | ATOM | 3724 | CG1 | ILE | A | 469 | 35.527 | 40.557 | 83.263 | 1.00 | 19.73 |
|    | ATOM | 3725 | CG2 | ILE | A | 469 | 36.688 | 40.791 | 85.497 | 1.00 | 11.46 |
|    | ATOM | 3726 | CD1 | ILE | A | 469 | 35.788 | 39.073 | 82.977 | 1.00 | 25.13 |
| 30 | ATOM | 3727 | N   | ALA | A | 470 | 38.776 | 43.375 | 84.572 | 1.00 | 12.77 |
|    | ATOM | 3728 | CA  | ALA | A | 470 | 39.729 | 43.967 | 85.475 | 1.00 | 11.93 |
|    | ATOM | 3729 | C   | ALA | A | 470 | 39.304 | 45.404 | 85.786 | 1.00 | 14.05 |
|    | ATOM | 3730 | O   | ALA | A | 470 | 39.264 | 45.860 | 86.941 | 1.00 | 15.14 |
|    | ATOM | 3731 | CB  | ALA | A | 470 | 41.078 | 43.982 | 84.759 | 1.00 | 12.54 |
| 35 | ATOM | 3732 | N   | LEU | A | 471 | 38.979 | 46.120 | 84.708 | 1.00 | 15.25 |
|    | ATOM | 3733 | CA  | LEU | A | 471 | 38.585 | 47.538 | 84.796 | 1.00 | 13.62 |
|    | ATOM | 3734 | C   | LEU | A | 471 | 37.257 | 47.792 | 85.510 | 1.00 | 17.64 |
|    | ATOM | 3735 | O   | LEU | A | 471 | 37.144 | 48.630 | 86.411 | 1.00 | 13.08 |
|    | ATOM | 3736 | CB  | LEU | A | 471 | 38.685 | 48.274 | 83.442 | 1.00 | 11.79 |
| 40 | ATOM | 3737 | CG  | LEU | A | 471 | 38.684 | 49.803 | 83.614 | 1.00 | 15.97 |
|    | ATOM | 3738 | CD1 | LEU | A | 471 | 39.855 | 50.262 | 84.497 | 1.00 | 12.47 |
|    | ATOM | 3739 | CD2 | LEU | A | 471 | 38.753 | 50.493 | 82.248 | 1.00 | 17.27 |
|    | ATOM | 3740 | N   | SER | A | 472 | 36.220 | 47.049 | 85.137 | 1.00 | 14.37 |
|    | ATOM | 3741 | CA  | SER | A | 472 | 34.963 | 47.264 | 85.808 | 1.00 | 11.84 |
| 45 | ATOM | 3742 | C   | SER | A | 472 | 35.082 | 46.900 | 87.284 | 1.00 | 18.13 |
|    | ATOM | 3743 | O   | SER | A | 472 | 34.533 | 47.581 | 88.145 | 1.00 | 16.29 |
|    | ATOM | 3744 | CB  | SER | A | 472 | 33.822 | 46.488 | 85.153 | 1.00 | 12.21 |
|    | ATOM | 3745 | OG  | SER | A | 472 | 34.090 | 45.121 | 85.240 | 1.00 | 18.74 |
|    | ATOM | 3746 | N   | GLN | A | 473 | 35.761 | 45.804 | 87.615 | 1.00 | 12.67 |
| 50 | ATOM | 3747 | CA  | GLN | A | 473 | 35.886 | 45.455 | 89.028 | 1.00 | 10.49 |
|    | ATOM | 3748 | C   | GLN | A | 473 | 36.615 | 46.538 | 89.813 | 1.00 | 12.50 |
|    | ATOM | 3749 | O   | GLN | A | 473 | 36.278 | 46.879 | 90.950 | 1.00 | 12.44 |
|    | ATOM | 3750 | CB  | GLN | A | 473 | 36.649 | 44.137 | 89.180 | 1.00 | 13.06 |
|    | ATOM | 3751 | CG  | GLN | A | 473 | 35.730 | 42.908 | 89.040 | 1.00 | 20.04 |
| 55 | ATOM | 3752 | CD  | GLN | A | 473 | 34.634 | 42.874 | 90.108 | 1.00 | 19.81 |
|    | ATOM | 3753 | OE1 | GLN | A | 473 | 34.917 | 42.605 | 91.270 | 1.00 | 30.46 |
|    | ATOM | 3754 | NE2 | GLN | A | 473 | 33.387 | 43.130 | 89.742 | 1.00 | 21.25 |
|    | ATOM | 3755 | N   | ARG | A | 474 | 37.656 | 47.087 | 89.183 | 1.00 | 14.11 |
|    | ATOM | 3756 | CA  | ARG | A | 474 | 38.400 | 48.158 | 89.868 | 1.00 | 17.39 |
| 60 | ATOM | 3757 | C   | ARG | A | 474 | 37.478 | 49.325 | 90.235 | 1.00 | 21.36 |
|    | ATOM | 3758 | O   | ARG | A | 474 | 37.577 | 49.922 | 91.304 | 1.00 | 18.76 |
|    | ATOM | 3759 | CB  | ARG | A | 474 | 39.532 | 48.719 | 89.034 | 1.00 | 11.27 |
|    | ATOM | 3760 | CG  | ARG | A | 474 | 40.786 | 47.842 | 89.038 | 1.00 | 17.88 |
|    | ATOM | 3761 | CD  | ARG | A | 474 | 41.727 | 48.283 | 87.928 | 1.00 | 21.70 |
|    | ATOM | 3762 | NE  | ARG | A | 474 | 42.122 | 49.665 | 88.177 | 1.00 | 19.49 |



|    |      |      |     |     |   |     |        |        |         |      |        |
|----|------|------|-----|-----|---|-----|--------|--------|---------|------|--------|
| 5  | ATOM | 3763 | CZ  | ARG | A | 474 | 42.837 | 50.419 | 87.361  | 1.00 | 31.34  |
|    | ATOM | 3764 | NH1 | ARG | A | 474 | 43.239 | 49.918 | 86.190  | 1.00 | 25.99  |
|    | ATOM | 3765 | NH2 | ARG | A | 474 | 43.160 | 51.679 | 87.742  | 1.00 | 17.92  |
|    | ATOM | 3766 | N   | TRP | A | 475 | 36.602 | 49.686 | 89.306  | 1.00 | 14.64  |
|    | ATOM | 3767 | CA  | TRP | A | 475 | 35.683 | 50.774 | 89.542  | 1.00 | 13.85  |
| 10 | ATOM | 3768 | C   | TRP | A | 475 | 34.608 | 50.352 | 90.524  | 1.00 | 18.33  |
|    | ATOM | 3769 | O   | TRP | A | 475 | 34.250 | 51.076 | 91.430  | 1.00 | 15.30  |
|    | ATOM | 3770 | CB  | TRP | A | 475 | 35.033 | 51.236 | 88.235  | 1.00 | 13.65  |
|    | ATOM | 3771 | CG  | TRP | A | 475 | 35.867 | 52.222 | 87.479  | 1.00 | 14.81  |
|    | ATOM | 3772 | CD1 | TRP | A | 475 | 36.645 | 51.943 | 86.399  | 1.00 | 17.78  |
| 15 | ATOM | 3773 | CD2 | TRP | A | 475 | 36.007 | 53.640 | 87.742  | 1.00 | 14.88  |
|    | ATOM | 3774 | NE1 | TRP | A | 475 | 37.284 | 53.090 | 85.976  | 1.00 | 18.25  |
|    | ATOM | 3775 | CE2 | TRP | A | 475 | 36.885 | 54.152 | 86.756  | 1.00 | 20.66  |
|    | ATOM | 3776 | CE3 | TRP | A | 475 | 35.464 | 54.518 | 88.694  | 1.00 | 15.98  |
|    | ATOM | 3777 | CZ2 | TRP | A | 475 | 37.243 | 55.511 | 86.714  | 1.00 | 19.78  |
| 20 | ATOM | 3778 | CZ3 | TRP | A | 475 | 35.839 | 55.853 | 88.665  | 1.00 | 18.27  |
|    | ATOM | 3779 | CH2 | TRP | A | 475 | 36.723 | 56.341 | 87.682  | 1.00 | 18.20  |
|    | ATOM | 3780 | N   | ILE | A | 476 | 34.081 | 49.157 | 90.362  | 1.00 | 15.43  |
|    | ATOM | 3781 | CA  | ILE | A | 476 | 33.027 | 48.713 | 91.251  | 1.00 | 15.88  |
|    | ATOM | 3782 | C   | ILE | A | 476 | 33.508 | 48.628 | 92.684  | 1.00 | 21.66  |
| 25 | ATOM | 3783 | O   | ILE | A | 476 | 32.742 | 48.833 | 93.614  | 1.00 | 20.18  |
|    | ATOM | 3784 | CB  | ILE | A | 476 | 32.498 | 47.354 | 90.775  | 1.00 | 16.74  |
|    | ATOM | 3785 | CG1 | ILE | A | 476 | 31.692 | 47.485 | 89.497  | 1.00 | 13.74  |
|    | ATOM | 3786 | CG2 | ILE | A | 476 | 31.697 | 46.620 | 91.844  | 1.00 | 17.08  |
|    | ATOM | 3787 | CD1 | ILE | A | 476 | 31.568 | 46.130 | 88.810  | 1.00 | 22.82  |
| 30 | ATOM | 3788 | N   | THR | A | 477 | 34.780 | 48.321 | 92.886  | 1.00 | 18.89  |
|    | ATOM | 3789 | CA  | THR | A | 477 | 35.286 | 48.193 | 94.256  | 1.00 | 15.92  |
|    | ATOM | 3790 | C   | THR | A | 477 | 36.151 | 49.355 | 94.708  | 1.00 | 17.65  |
|    | ATOM | 3791 | O   | THR | A | 477 | 36.711 | 49.333 | 95.792  | 1.00 | 17.49  |
|    | ATOM | 3792 | CB  | THR | A | 477 | 36.132 | 46.904 | 94.384  | 1.00 | 21.13  |
| 35 | ATOM | 3793 | OG1 | THR | A | 477 | 37.296 | 46.986 | 93.545  | 1.00 | 19.88  |
|    | ATOM | 3794 | CG2 | THR | A | 477 | 35.268 | 45.673 | 94.035  | 1.00 | 16.31  |
|    | ATOM | 3795 | N   | ALA | A | 478 | 36.302 | 50.369 | 93.884  | 1.00 | 18.44  |
|    | ATOM | 3796 | CA  | ALA | A | 478 | 37.131 | 51.548 | 94.191  | 1.00 | 16.94  |
|    | ATOM | 3797 | C   | ALA | A | 478 | 36.729 | 52.219 | 95.490  | 1.00 | 20.18  |
| 40 | ATOM | 3798 | O   | ALA | A | 478 | 35.552 | 52.233 | 95.863  | 1.00 | 19.40  |
|    | ATOM | 3799 | CB  | ALA | A | 478 | 37.017 | 52.608 | 93.077  | 1.00 | 15.66  |
|    | ATOM | 3800 | N   | LYS | A | 479 | 37.753 | 52.763 | 96.148  | 1.00 | 17.33  |
|    | ATOM | 3801 | CA  | LYS | A | 479 | 37.654 | 53.518 | 97.371  | 1.00 | 15.43  |
|    | ATOM | 3802 | C   | LYS | A | 479 | 38.196 | 54.907 | 97.115  | 1.00 | 19.77  |
| 45 | ATOM | 3803 | O   | LYS | A | 479 | 38.757 | 55.192 | 96.073  | 1.00 | 16.97  |
|    | ATOM | 3804 | CB  | LYS | A | 479 | 38.325 | 52.853 | 98.562  | 1.00 | 17.71  |
|    | ATOM | 3805 | CG  | LYS | A | 479 | 37.468 | 51.685 | 99.049  | 1.00 | 25.29  |
|    | ATOM | 3806 | CD  | LYS | A | 479 | 38.002 | 51.058 | 100.324 | 1.00 | 28.77  |
|    | ATOM | 3807 | CE  | LYS | A | 479 | 36.895 | 50.623 | 101.280 | 1.00 | 75.63  |
| 50 | ATOM | 3808 | NZ  | LYS | A | 479 | 36.090 | 49.481 | 100.815 | 1.00 | 66.83  |
|    | ATOM | 3809 | N   | GLU | A | 480 | 38.010 | 55.793 | 98.068  | 1.00 | 19.41  |
|    | ATOM | 3810 | CA  | GLU | A | 480 | 38.497 | 57.120 | 97.853  | 1.00 | 19.30  |
|    | ATOM | 3811 | C   | GLU | A | 480 | 39.933 | 57.069 | 97.387  | 1.00 | 21.25  |
|    | ATOM | 3812 | O   | GLU | A | 480 | 40.321 | 57.802 | 96.489  | 1.00 | 21.38  |
| 55 | ATOM | 3813 | CB  | GLU | A | 480 | 38.457 | 57.901 | 99.183  | 1.00 | 21.20  |
|    | ATOM | 3814 | CG  | GLU | A | 480 | 37.322 | 58.931 | 99.171  | 1.00 | 53.93  |
|    | ATOM | 3815 | CD  | GLU | A | 480 | 37.505 | 59.998 | 98.131  | 1.00 | 100.00 |
|    | ATOM | 3816 | OE1 | GLU | A | 480 | 38.596 | 60.401 | 97.756  | 1.00 | 100.00 |
|    | ATOM | 3817 | OE2 | GLU | A | 480 | 36.360 | 60.456 | 97.684  | 1.00 | 100.00 |
| 60 | ATOM | 3818 | N   | ASP | A | 481 | 40.730 | 56.249 | 98.059  | 1.00 | 15.59  |
|    | ATOM | 3819 | CA  | ASP | A | 481 | 42.120 | 56.150 | 97.734  | 1.00 | 17.58  |
|    | ATOM | 3820 | C   | ASP | A | 481 | 42.463 | 55.609 | 96.372  | 1.00 | 22.00  |
|    | ATOM | 3821 | O   | ASP | A | 481 | 43.639 | 55.651 | 96.002  | 1.00 | 21.23  |
|    | ATOM | 3822 | CB  | ASP | A | 481 | 42.966 | 55.475 | 98.824  | 1.00 | 22.35  |
|    | ATOM | 3823 | CG  | ASP | A | 481 | 42.845 | 53.974 | 98.879  | 1.00 | 26.70  |
|    | ATOM | 3824 | OD1 | ASP | A | 481 | 42.040 | 53.276 | 98.295  | 1.00 | 22.31  |
|    | ATOM | 3825 | OD2 | ASP | A | 481 | 43.769 | 53.466 | 99.638  | 1.00 | 19.37  |
|    | ATOM | 3826 | N   | ASP | A | 482 | 41.483 | 55.147 | 95.608  | 1.00 | 16.23  |



|    |      |      |     |     |   |     |        |        |        |      |        |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
|    | ATOM | 3827 | CA  | ASP | A | 482 | 41.795 | 54.667 | 94.250 | 1.00 | 15.66  |
|    | ATOM | 3828 | C   | ASP | A | 482 | 41.485 | 55.667 | 93.144 | 1.00 | 20.38  |
|    | ATOM | 3829 | O   | ASP | A | 482 | 41.994 | 55.549 | 92.031 | 1.00 | 19.78  |
| 5  | ATOM | 3830 | CB  | ASP | A | 482 | 41.058 | 53.340 | 93.885 | 1.00 | 16.37  |
|    | ATOM | 3831 | CG  | ASP | A | 482 | 41.360 | 52.283 | 94.918 | 1.00 | 14.59  |
|    | ATOM | 3832 | OD1 | ASP | A | 482 | 42.463 | 51.867 | 95.146 | 1.00 | 16.94  |
|    | ATOM | 3833 | OD2 | ASP | A | 482 | 40.338 | 51.972 | 95.654 | 1.00 | 17.55  |
|    | ATOM | 3834 | N   | LEU | A | 483 | 40.627 | 56.645 | 93.423 | 1.00 | 17.94  |
| 10 | ATOM | 3835 | CA  | LEU | A | 483 | 40.167 | 57.591 | 92.403 | 1.00 | 14.70  |
|    | ATOM | 3836 | C   | LEU | A | 483 | 41.214 | 58.319 | 91.581 | 1.00 | 21.17  |
|    | ATOM | 3837 | O   | LEU | A | 483 | 41.122 | 58.519 | 90.368 | 1.00 | 21.03  |
|    | ATOM | 3838 | CB  | LEU | A | 483 | 39.110 | 58.581 | 92.960 | 1.00 | 13.43  |
|    | ATOM | 3839 | CG  | LEU | A | 483 | 37.870 | 57.925 | 93.558 | 1.00 | 15.53  |
| 15 | ATOM | 3840 | CD1 | LEU | A | 483 | 36.970 | 59.020 | 94.114 | 1.00 | 19.32  |
|    | ATOM | 3841 | CD2 | LEU | A | 483 | 37.047 | 57.172 | 92.512 | 1.00 | 16.27  |
|    | ATOM | 3842 | N   | ASN | A | 484 | 42.220 | 58.761 | 92.289 | 1.00 | 19.63  |
|    | ATOM | 3843 | CA  | ASN | A | 484 | 43.274 | 59.541 | 91.713 | 1.00 | 19.74  |
|    | ATOM | 3844 | C   | ASN | A | 484 | 44.128 | 58.789 | 90.738 | 1.00 | 21.84  |
| 20 | ATOM | 3845 | O   | ASN | A | 484 | 44.723 | 59.343 | 89.827 | 1.00 | 20.30  |
|    | ATOM | 3846 | CB  | ASN | A | 484 | 44.110 | 60.036 | 92.891 | 1.00 | 34.83  |
|    | ATOM | 3847 | CG  | ASN | A | 484 | 45.382 | 60.719 | 92.449 | 1.00 | 100.00 |
|    | ATOM | 3848 | OD1 | ASN | A | 484 | 45.345 | 61.686 | 91.662 | 1.00 | 87.99  |
|    | ATOM | 3849 | ND2 | ASN | A | 484 | 46.510 | 60.200 | 92.946 | 1.00 | 100.00 |
| 25 | ATOM | 3850 | N   | SER | A | 485 | 44.183 | 57.510 | 90.918 | 1.00 | 17.69  |
|    | ATOM | 3851 | CA  | SER | A | 485 | 44.986 | 56.711 | 90.020 | 1.00 | 19.64  |
|    | ATOM | 3852 | C   | SER | A | 485 | 44.283 | 56.335 | 88.728 | 1.00 | 22.88  |
|    | ATOM | 3853 | O   | SER | A | 485 | 44.965 | 55.937 | 87.778 | 1.00 | 23.74  |
|    | ATOM | 3854 | CB  | SER | A | 485 | 45.543 | 55.508 | 90.752 | 1.00 | 26.03  |
| 30 | ATOM | 3855 | OG  | SER | A | 485 | 45.864 | 55.954 | 92.057 | 1.00 | 52.22  |
|    | ATOM | 3856 | N   | PHE | A | 486 | 42.948 | 56.451 | 88.650 | 1.00 | 15.68  |
|    | ATOM | 3857 | CA  | PHE | A | 486 | 42.367 | 56.105 | 87.371 | 1.00 | 17.12  |
|    | ATOM | 3858 | C   | PHE | A | 486 | 42.879 | 57.120 | 86.403 | 1.00 | 16.98  |
|    | ATOM | 3859 | O   | PHE | A | 486 | 43.165 | 58.236 | 86.812 | 1.00 | 15.87  |
| 35 | ATOM | 3860 | CB  | PHE | A | 486 | 40.827 | 56.088 | 87.376 | 1.00 | 18.47  |
|    | ATOM | 3861 | CG  | PHE | A | 486 | 40.270 | 54.950 | 88.181 | 1.00 | 17.85  |
|    | ATOM | 3862 | CD1 | PHE | A | 486 | 40.325 | 53.646 | 87.686 | 1.00 | 17.48  |
|    | ATOM | 3863 | CD2 | PHE | A | 486 | 39.669 | 55.169 | 89.423 | 1.00 | 19.85  |
|    | ATOM | 3864 | CE1 | PHE | A | 486 | 39.790 | 52.599 | 88.441 | 1.00 | 18.74  |
| 40 | ATOM | 3865 | CE2 | PHE | A | 486 | 39.119 | 54.139 | 90.189 | 1.00 | 19.10  |
|    | ATOM | 3866 | CZ  | PHE | A | 486 | 39.208 | 52.839 | 89.689 | 1.00 | 17.75  |
|    | ATOM | 3867 | N   | ASN | A | 487 | 42.965 | 56.744 | 85.140 | 1.00 | 16.22  |
|    | ATOM | 3868 | CA  | ASN | A | 487 | 43.499 | 57.636 | 84.141 | 1.00 | 20.09  |
|    | ATOM | 3869 | C   | ASN | A | 487 | 43.100 | 57.184 | 82.746 | 1.00 | 23.67  |
| 45 | ATOM | 3870 | O   | ASN | A | 487 | 42.770 | 56.024 | 82.522 | 1.00 | 22.60  |
|    | ATOM | 3871 | CB  | ASN | A | 487 | 45.058 | 57.575 | 84.255 | 1.00 | 21.63  |
|    | ATOM | 3872 | CG  | ASN | A | 487 | 45.776 | 58.616 | 83.415 | 1.00 | 32.80  |
|    | ATOM | 3873 | OD1 | ASN | A | 487 | 45.901 | 58.498 | 82.202 | 1.00 | 29.22  |
|    | ATOM | 3874 | ND2 | ASN | A | 487 | 46.159 | 59.725 | 84.021 | 1.00 | 31.52  |
| 50 | ATOM | 3875 | N   | ALA | A | 488 | 43.145 | 58.126 | 81.800 | 1.00 | 23.87  |
|    | ATOM | 3876 | CA  | ALA | A | 488 | 42.808 | 57.829 | 80.411 | 1.00 | 24.07  |
|    | ATOM | 3877 | C   | ALA | A | 488 | 43.673 | 56.703 | 79.873 | 1.00 | 30.63  |
|    | ATOM | 3878 | O   | ALA | A | 488 | 43.336 | 55.962 | 78.958 | 1.00 | 33.83  |
|    | ATOM | 3879 | CB  | ALA | A | 488 | 42.978 | 59.086 | 79.574 | 1.00 | 26.14  |
| 55 | ATOM | 3880 | N   | THR | A | 489 | 44.835 | 56.532 | 80.467 | 1.00 | 25.63  |
|    | ATOM | 3881 | CA  | THR | A | 489 | 45.666 | 55.468 | 79.987 | 1.00 | 22.82  |
|    | ATOM | 3882 | C   | THR | A | 489 | 44.976 | 54.168 | 80.210 | 1.00 | 24.75  |
|    | ATOM | 3883 | O   | THR | A | 489 | 45.323 | 53.163 | 79.615 | 1.00 | 26.26  |
|    | ATOM | 3884 | CB  | THR | A | 489 | 47.017 | 55.459 | 80.691 | 1.00 | 29.64  |
| 60 | ATOM | 3885 | OG1 | THR | A | 489 | 46.814 | 55.537 | 82.076 | 1.00 | 29.43  |
|    | ATOM | 3886 | CG2 | THR | A | 489 | 47.774 | 56.684 | 80.231 | 1.00 | 35.78  |
|    | ATOM | 3887 | N   | ASP | A | 490 | 43.999 | 54.180 | 81.097 | 1.00 | 21.60  |
|    | ATOM | 3888 | CA  | ASP | A | 490 | 43.288 | 52.946 | 81.362 | 1.00 | 20.54  |
|    | ATOM | 3889 | C   | ASP | A | 490 | 42.628 | 52.391 | 80.104 | 1.00 | 14.90  |
|    | ATOM | 3890 | O   | ASP | A | 490 | 42.363 | 51.207 | 80.013 | 1.00 | 18.94  |



|    |      |      |     |     |   |     |        |        |        |      |        |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
|    | ATOM | 3891 | CB  | ASP | A | 490 | 42.188 | 53.100 | 82.462 | 1.00 | 18.42  |
|    | ATOM | 3892 | CG  | ASP | A | 490 | 42.764 | 53.483 | 83.785 | 1.00 | 21.60  |
|    | ATOM | 3893 | OD1 | ASP | A | 490 | 43.865 | 53.165 | 84.170 | 1.00 | 22.97  |
| 5  | ATOM | 3894 | OD2 | ASP | A | 490 | 41.930 | 54.124 | 84.534 | 1.00 | 18.24  |
|    | ATOM | 3895 | N   | LEU | A | 491 | 42.309 | 53.262 | 79.180 | 1.00 | 14.42  |
|    | ATOM | 3896 | CA  | LEU | A | 491 | 41.571 | 52.910 | 77.971 | 1.00 | 18.63  |
|    | ATOM | 3897 | C   | LEU | A | 491 | 42.404 | 52.634 | 76.735 | 1.00 | 26.17  |
|    | ATOM | 3898 | O   | LEU | A | 491 | 41.863 | 52.350 | 75.689 | 1.00 | 23.53  |
| 10 | ATOM | 3899 | CB  | LEU | A | 491 | 40.626 | 54.065 | 77.600 | 1.00 | 16.48  |
|    | ATOM | 3900 | CG  | LEU | A | 491 | 39.793 | 54.553 | 78.786 | 1.00 | 17.62  |
|    | ATOM | 3901 | CD1 | LEU | A | 491 | 38.719 | 55.504 | 78.256 | 1.00 | 18.61  |
|    | ATOM | 3902 | CD2 | LEU | A | 491 | 39.164 | 53.341 | 79.481 | 1.00 | 10.99  |
|    | ATOM | 3903 | N   | LYS | A | 492 | 43.697 | 52.773 | 76.906 | 1.00 | 25.72  |
| 15 | ATOM | 3904 | CA  | LYS | A | 492 | 44.773 | 52.625 | 75.944 | 1.00 | 29.38  |
|    | ATOM | 3905 | C   | LYS | A | 492 | 44.601 | 51.464 | 74.987 | 1.00 | 26.62  |
|    | ATOM | 3906 | O   | LYS | A | 492 | 44.640 | 51.598 | 73.769 | 1.00 | 25.36  |
|    | ATOM | 3907 | CB  | LYS | A | 492 | 46.051 | 52.369 | 76.768 | 1.00 | 39.68  |
|    | ATOM | 3908 | CG  | LYS | A | 492 | 47.400 | 52.731 | 76.164 | 1.00 | 74.03  |
| 20 | ATOM | 3909 | CD  | LYS | A | 492 | 48.535 | 52.573 | 77.175 | 1.00 | 92.88  |
|    | ATOM | 3910 | CE  | LYS | A | 492 | 49.162 | 51.184 | 77.249 | 1.00 | 100.00 |
|    | ATOM | 3911 | NZ  | LYS | A | 492 | 50.629 | 51.214 | 77.397 | 1.00 | 100.00 |
|    | ATOM | 3912 | N   | ASP | A | 493 | 44.504 | 50.271 | 75.514 | 1.00 | 22.05  |
|    | ATOM | 3913 | CA  | ASP | A | 493 | 44.400 | 49.213 | 74.525 | 1.00 | 25.28  |
| 25 | ATOM | 3914 | C   | ASP | A | 493 | 43.008 | 48.604 | 74.421 | 1.00 | 31.85  |
|    | ATOM | 3915 | O   | ASP | A | 493 | 42.844 | 47.411 | 74.178 | 1.00 | 31.64  |
|    | ATOM | 3916 | CB  | ASP | A | 493 | 45.414 | 48.126 | 74.874 | 1.00 | 30.29  |
|    | ATOM | 3917 | CG  | ASP | A | 493 | 46.803 | 48.680 | 74.973 | 1.00 | 47.27  |
|    | ATOM | 3918 | OD1 | ASP | A | 493 | 47.322 | 49.280 | 74.036 | 1.00 | 49.99  |
| 30 | ATOM | 3919 | OD2 | ASP | A | 493 | 47.334 | 48.481 | 76.167 | 1.00 | 45.03  |
|    | ATOM | 3920 | N   | LEU | A | 494 | 41.989 | 49.430 | 74.622 | 1.00 | 23.95  |
|    | ATOM | 3921 | CA  | LEU | A | 494 | 40.633 | 48.920 | 74.576 | 1.00 | 19.08  |
|    | ATOM | 3922 | C   | LEU | A | 494 | 39.939 | 49.350 | 73.295 | 1.00 | 21.27  |
|    | ATOM | 3923 | O   | LEU | A | 494 | 39.960 | 50.537 | 72.963 | 1.00 | 22.24  |
| 35 | ATOM | 3924 | CB  | LEU | A | 494 | 39.833 | 49.421 | 75.800 | 1.00 | 16.85  |
|    | ATOM | 3925 | CG  | LEU | A | 494 | 40.346 | 48.949 | 77.145 | 1.00 | 19.46  |
|    | ATOM | 3926 | CD1 | LEU | A | 494 | 39.307 | 49.363 | 78.182 | 1.00 | 18.39  |
|    | ATOM | 3927 | CD2 | LEU | A | 494 | 40.511 | 47.422 | 77.183 | 1.00 | 20.77  |
|    | ATOM | 3928 | N   | SER | A | 495 | 39.320 | 48.401 | 72.573 | 1.00 | 17.36  |
| 40 | ATOM | 3929 | CA  | SER | A | 495 | 38.594 | 48.790 | 71.382 | 1.00 | 16.04  |
|    | ATOM | 3930 | C   | SER | A | 495 | 37.256 | 49.395 | 71.854 | 1.00 | 16.87  |
|    | ATOM | 3931 | O   | SER | A | 495 | 36.902 | 49.328 | 73.042 | 1.00 | 13.30  |
|    | ATOM | 3932 | CB  | SER | A | 495 | 38.253 | 47.547 | 70.576 | 1.00 | 16.67  |
|    | ATOM | 3933 | OG  | SER | A | 495 | 37.477 | 46.701 | 71.422 | 1.00 | 17.37  |
| 45 | ATOM | 3934 | N   | SER | A | 496 | 36.496 | 49.950 | 70.922 | 1.00 | 14.14  |
|    | ATOM | 3935 | CA  | SER | A | 496 | 35.200 | 50.501 | 71.254 | 1.00 | 16.64  |
|    | ATOM | 3936 | C   | SER | A | 496 | 34.316 | 49.365 | 71.794 | 1.00 | 17.90  |
|    | ATOM | 3937 | O   | SER | A | 496 | 33.495 | 49.589 | 72.680 | 1.00 | 16.25  |
|    | ATOM | 3938 | CB  | SER | A | 496 | 34.553 | 51.190 | 70.050 | 1.00 | 17.35  |
| 50 | ATOM | 3939 | OG  | SER | A | 496 | 34.309 | 50.183 | 69.105 | 1.00 | 23.79  |
|    | ATOM | 3940 | N   | HIS | A | 497 | 34.522 | 48.136 | 71.274 | 1.00 | 15.34  |
|    | ATOM | 3941 | CA  | HIS | A | 497 | 33.794 | 46.965 | 71.729 | 1.00 | 13.46  |
|    | ATOM | 3942 | C   | HIS | A | 497 | 33.999 | 46.671 | 73.224 | 1.00 | 17.45  |
|    | ATOM | 3943 | O   | HIS | A | 497 | 33.120 | 46.277 | 73.992 | 1.00 | 17.69  |
| 55 | ATOM | 3944 | CB  | HIS | A | 497 | 34.211 | 45.761 | 70.874 | 1.00 | 13.79  |
|    | ATOM | 3945 | CG  | HIS | A | 497 | 33.804 | 46.004 | 69.470 | 1.00 | 20.43  |
|    | ATOM | 3946 | ND1 | HIS | A | 497 | 34.738 | 46.342 | 68.482 | 1.00 | 24.52  |
|    | ATOM | 3947 | CD2 | HIS | A | 497 | 32.551 | 46.044 | 68.930 | 1.00 | 21.08  |
|    | ATOM | 3948 | CE1 | HIS | A | 497 | 34.039 | 46.531 | 67.358 | 1.00 | 21.87  |
| 60 | ATOM | 3949 | NE2 | HIS | A | 497 | 32.725 | 46.363 | 67.602 | 1.00 | 23.02  |
|    | ATOM | 3950 | N   | GLN | A | 498 | 35.230 | 46.833 | 73.662 | 1.00 | 14.00  |
|    | ATOM | 3951 | CA  | GLN | A | 498 | 35.633 | 46.593 | 75.029 | 1.00 | 10.78  |
|    | ATOM | 3952 | C   | GLN | A | 498 | 35.180 | 47.697 | 75.968 | 1.00 | 13.63  |
|    | ATOM | 3953 | O   | GLN | A | 498 | 34.829 | 47.449 | 77.118 | 1.00 | 13.35  |
|    | ATOM | 3954 | CB  | GLN | A | 498 | 37.156 | 46.416 | 75.038 | 1.00 | 11.59  |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
|    | ATOM | 3955 | CG  | GLN | A | 498 | 37.585 | 45.026 | 74.488 | 1.00 | 14.99 |
|    | ATOM | 3956 | CD  | GLN | A | 498 | 39.101 | 44.938 | 74.454 | 1.00 | 21.92 |
|    | ATOM | 3957 | OE1 | GLN | A | 498 | 39.746 | 45.833 | 73.897 | 1.00 | 18.12 |
| 5  | ATOM | 3958 | NE2 | GLN | A | 498 | 39.685 | 43.957 | 75.117 | 1.00 | 11.55 |
|    | ATOM | 3959 | N   | LEU | A | 499 | 35.200 | 48.942 | 75.490 | 1.00 | 16.63 |
|    | ATOM | 3960 | CA  | LEU | A | 499 | 34.712 | 50.095 | 76.273 | 1.00 | 18.30 |
|    | ATOM | 3961 | C   | LEU | A | 499 | 33.222 | 49.848 | 76.647 | 1.00 | 18.08 |
|    | ATOM | 3962 | O   | LEU | A | 499 | 32.711 | 50.004 | 77.782 | 1.00 | 14.69 |
| 10 | ATOM | 3963 | CB  | LEU | A | 499 | 34.719 | 51.296 | 75.293 | 1.00 | 19.02 |
|    | ATOM | 3964 | CG  | LEU | A | 499 | 35.650 | 52.421 | 75.677 | 1.00 | 28.28 |
|    | ATOM | 3965 | CD1 | LEU | A | 499 | 36.768 | 51.856 | 76.527 | 1.00 | 27.69 |
|    | ATOM | 3966 | CD2 | LEU | A | 499 | 36.210 | 53.135 | 74.448 | 1.00 | 31.77 |
|    | ATOM | 3967 | N   | ASN | A | 500 | 32.491 | 49.430 | 75.610 | 1.00 | 11.59 |
| 15 | ATOM | 3968 | CA  | ASN | A | 500 | 31.084 | 49.123 | 75.748 | 1.00 | 10.98 |
|    | ATOM | 3969 | C   | ASN | A | 500 | 30.844 | 48.021 | 76.775 | 1.00 | 11.55 |
|    | ATOM | 3970 | O   | ASN | A | 500 | 29.989 | 48.125 | 77.656 | 1.00 | 13.43 |
|    | ATOM | 3971 | CB  | ASN | A | 500 | 30.530 | 48.735 | 74.355 | 1.00 | 11.90 |
|    | ATOM | 3972 | CG  | ASN | A | 500 | 29.020 | 48.504 | 74.328 | 1.00 | 26.05 |
| 20 | ATOM | 3973 | OD1 | ASN | A | 500 | 28.208 | 49.304 | 74.815 | 1.00 | 19.55 |
|    | ATOM | 3974 | ND2 | ASN | A | 500 | 28.607 | 47.387 | 73.759 | 1.00 | 21.02 |
|    | ATOM | 3975 | N   | GLU | A | 501 | 31.601 | 46.927 | 76.633 | 1.00 | 11.18 |
|    | ATOM | 3976 | CA  | GLU | A | 501 | 31.471 | 45.787 | 77.537 | 1.00 | 11.00 |
|    | ATOM | 3977 | C   | GLU | A | 501 | 31.859 | 46.184 | 78.954 | 1.00 | 14.40 |
| 25 | ATOM | 3978 | O   | GLU | A | 501 | 31.266 | 45.757 | 79.930 | 1.00 | 13.70 |
|    | ATOM | 3979 | CB  | GLU | A | 501 | 32.286 | 44.574 | 77.022 | 1.00 | 13.23 |
|    | ATOM | 3980 | CG  | GLU | A | 501 | 32.328 | 43.425 | 78.064 | 1.00 | 12.24 |
|    | ATOM | 3981 | CD  | GLU | A | 501 | 30.930 | 42.880 | 78.253 | 1.00 | 20.51 |
|    | ATOM | 3982 | OE1 | GLU | A | 501 | 30.040 | 43.113 | 77.452 | 1.00 | 18.75 |
| 30 | ATOM | 3983 | OE2 | GLU | A | 501 | 30.747 | 42.158 | 79.338 | 1.00 | 16.17 |
|    | ATOM | 3984 | N   | PHE | A | 502 | 32.876 | 47.051 | 79.080 | 1.00 | 10.99 |
|    | ATOM | 3985 | CA  | PHE | A | 502 | 33.281 | 47.530 | 80.382 | 1.00 | 12.47 |
|    | ATOM | 3986 | C   | PHE | A | 502 | 32.095 | 48.241 | 81.068 | 1.00 | 12.80 |
|    | ATOM | 3987 | O   | PHE | A | 502 | 31.733 | 48.062 | 82.230 | 1.00 | 11.74 |
| 35 | ATOM | 3988 | CB  | PHE | A | 502 | 34.498 | 48.490 | 80.167 | 1.00 | 14.11 |
|    | ATOM | 3989 | CG  | PHE | A | 502 | 34.641 | 49.500 | 81.265 | 1.00 | 11.76 |
|    | ATOM | 3990 | CD1 | PHE | A | 502 | 34.958 | 49.120 | 82.570 | 1.00 | 9.77  |
|    | ATOM | 3991 | CD2 | PHE | A | 502 | 34.363 | 50.847 | 81.040 | 1.00 | 17.45 |
|    | ATOM | 3992 | CE1 | PHE | A | 502 | 35.059 | 50.053 | 83.605 | 1.00 | 12.88 |
| 40 | ATOM | 3993 | CE2 | PHE | A | 502 | 34.443 | 51.799 | 82.063 | 1.00 | 20.32 |
|    | ATOM | 3994 | CZ  | PHE | A | 502 | 34.812 | 51.406 | 83.350 | 1.00 | 16.55 |
|    | ATOM | 3995 | N   | LEU | A | 503 | 31.470 | 49.100 | 80.286 | 1.00 | 10.48 |
|    | ATOM | 3996 | CA  | LEU | A | 503 | 30.342 | 49.835 | 80.759 | 1.00 | 11.84 |
|    | ATOM | 3997 | C   | LEU | A | 503 | 29.184 | 48.917 | 81.089 | 1.00 | 11.65 |
| 45 | ATOM | 3998 | O   | LEU | A | 503 | 28.531 | 49.077 | 82.110 | 1.00 | 14.41 |
|    | ATOM | 3999 | CB  | LEU | A | 503 | 29.974 | 50.854 | 79.668 | 1.00 | 12.15 |
|    | ATOM | 4000 | CG  | LEU | A | 503 | 30.872 | 52.105 | 79.668 | 1.00 | 12.97 |
|    | ATOM | 4001 | CD1 | LEU | A | 503 | 30.572 | 52.957 | 78.438 | 1.00 | 9.62  |
|    | ATOM | 4002 | CD2 | LEU | A | 503 | 30.614 | 52.935 | 80.936 | 1.00 | 14.08 |
| 50 | ATOM | 4003 | N   | ALA | A | 504 | 28.947 | 47.910 | 80.248 | 1.00 | 12.65 |
|    | ATOM | 4004 | CA  | ALA | A | 504 | 27.850 | 46.977 | 80.499 | 1.00 | 8.77  |
|    | ATOM | 4005 | C   | ALA | A | 504 | 28.038 | 46.282 | 81.812 | 1.00 | 12.09 |
|    | ATOM | 4006 | O   | ALA | A | 504 | 27.118 | 46.081 | 82.598 | 1.00 | 10.26 |
|    | ATOM | 4007 | CB  | ALA | A | 504 | 27.742 | 45.965 | 79.370 | 1.00 | 7.47  |
| 55 | ATOM | 4008 | N   | GLN | A | 505 | 29.280 | 45.900 | 82.035 | 1.00 | 12.47 |
|    | ATOM | 4009 | CA  | GLN | A | 505 | 29.609 | 45.209 | 83.271 | 1.00 | 12.94 |
|    | ATOM | 4010 | C   | GLN | A | 505 | 29.424 | 46.144 | 84.484 | 1.00 | 14.71 |
|    | ATOM | 4011 | O   | GLN | A | 505 | 28.902 | 45.773 | 85.566 | 1.00 | 13.04 |
|    | ATOM | 4012 | CB  | GLN | A | 505 | 31.068 | 44.689 | 83.183 | 1.00 | 14.37 |
| 60 | ATOM | 4013 | CG  | GLN | A | 505 | 31.243 | 43.520 | 82.174 | 1.00 | 17.48 |
|    | ATOM | 4014 | CD  | GLN | A | 505 | 32.693 | 43.054 | 82.089 | 1.00 | 20.84 |
|    | ATOM | 4015 | OE1 | GLN | A | 505 | 33.556 | 43.462 | 82.890 | 1.00 | 21.65 |
|    | ATOM | 4016 | NE2 | GLN | A | 505 | 32.990 | 42.221 | 81.096 | 1.00 | 16.13 |
|    | ATOM | 4017 | N   | THR | A | 506 | 29.862 | 47.389 | 84.298 | 1.00 | 13.56 |
|    | ATOM | 4018 | CA  | THR | A | 506 | 29.749 | 48.348 | 85.373 | 1.00 | 15.13 |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
|    | ATOM | 4019 | C   | THR | A | 506 | 28.280 | 48.610 | 85.714 | 1.00 | 17.30 |
|    | ATOM | 4020 | O   | THR | A | 506 | 27.835 | 48.662 | 86.879 | 1.00 | 13.71 |
|    | ATOM | 4021 | CB  | THR | A | 506 | 30.561 | 49.613 | 85.043 | 1.00 | 13.74 |
| 5  | ATOM | 4022 | OG1 | THR | A | 506 | 31.903 | 49.243 | 84.853 | 1.00 | 13.66 |
|    | ATOM | 4023 | CG2 | THR | A | 506 | 30.542 | 50.538 | 86.242 | 1.00 | 16.98 |
|    | ATOM | 4024 | N   | LEU | A | 507 | 27.532 | 48.734 | 84.636 | 1.00 | 15.17 |
|    | ATOM | 4025 | CA  | LEU | A | 507 | 26.109 | 49.007 | 84.748 | 1.00 | 15.46 |
|    | ATOM | 4026 | C   | LEU | A | 507 | 25.391 | 47.944 | 85.517 | 1.00 | 15.53 |
| 10 | ATOM | 4027 | O   | LEU | A | 507 | 24.464 | 48.230 | 86.256 | 1.00 | 14.10 |
|    | ATOM | 4028 | CB  | LEU | A | 507 | 25.476 | 49.185 | 83.351 | 1.00 | 16.26 |
|    | ATOM | 4029 | CG  | LEU | A | 507 | 24.017 | 49.581 | 83.374 | 1.00 | 17.96 |
|    | ATOM | 4030 | CD1 | LEU | A | 507 | 23.801 | 50.929 | 84.087 | 1.00 | 12.71 |
|    | ATOM | 4031 | CD2 | LEU | A | 507 | 23.550 | 49.633 | 81.923 | 1.00 | 13.10 |
| 15 | ATOM | 4032 | N   | GLN | A | 508 | 25.802 | 46.696 | 85.343 | 1.00 | 14.24 |
|    | ATOM | 4033 | CA  | GLN | A | 508 | 25.145 | 45.630 | 86.077 | 1.00 | 11.70 |
|    | ATOM | 4034 | C   | GLN | A | 508 | 25.264 | 45.846 | 87.581 | 1.00 | 19.07 |
|    | ATOM | 4035 | O   | GLN | A | 508 | 24.521 | 45.269 | 88.354 | 1.00 | 16.98 |
|    | ATOM | 4036 | CB  | GLN | A | 508 | 25.736 | 44.246 | 85.745 | 1.00 | 11.79 |
| 20 | ATOM | 4037 | CG  | GLN | A | 508 | 25.402 | 43.722 | 84.334 | 1.00 | 17.73 |
|    | ATOM | 4038 | CD  | GLN | A | 508 | 25.860 | 42.282 | 84.204 | 1.00 | 20.08 |
|    | ATOM | 4039 | OE1 | GLN | A | 508 | 26.960 | 41.972 | 84.695 | 1.00 | 23.98 |
|    | ATOM | 4040 | NE2 | GLN | A | 508 | 25.048 | 41.402 | 83.594 | 1.00 | 15.23 |
|    | ATOM | 4041 | N   | ARG | A | 509 | 26.217 | 46.639 | 88.053 | 1.00 | 17.16 |
| 25 | ATOM | 4042 | CA  | ARG | A | 509 | 26.332 | 46.847 | 89.498 | 1.00 | 12.26 |
|    | ATOM | 4043 | C   | ARG | A | 509 | 25.960 | 48.279 | 89.899 | 1.00 | 17.09 |
|    | ATOM | 4044 | O   | ARG | A | 509 | 26.379 | 48.778 | 90.948 | 1.00 | 18.12 |
|    | ATOM | 4045 | CB  | ARG | A | 509 | 27.741 | 46.537 | 90.036 | 1.00 | 12.59 |
|    | ATOM | 4046 | CG  | ARG | A | 509 | 28.095 | 45.097 | 89.784 | 1.00 | 17.56 |
| 30 | ATOM | 4047 | CD  | ARG | A | 509 | 27.422 | 44.228 | 90.829 | 1.00 | 25.37 |
|    | ATOM | 4048 | NE  | ARG | A | 509 | 28.134 | 44.270 | 92.117 | 1.00 | 81.24 |
|    | ATOM | 4049 | CZ  | ARG | A | 509 | 29.377 | 43.822 | 92.417 | 1.00 | 88.85 |
|    | ATOM | 4050 | NH1 | ARG | A | 509 | 30.235 | 43.233 | 91.555 | 1.00 | 63.02 |
|    | ATOM | 4051 | NH2 | ARG | A | 509 | 29.779 | 43.978 | 93.676 | 1.00 | 42.33 |
| 35 | ATOM | 4052 | N   | ALA | A | 510 | 25.162 | 48.958 | 89.088 | 1.00 | 14.89 |
|    | ATOM | 4053 | CA  | ALA | A | 510 | 24.782 | 50.321 | 89.428 | 1.00 | 13.02 |
|    | ATOM | 4054 | C   | ALA | A | 510 | 23.824 | 50.270 | 90.594 | 1.00 | 22.66 |
|    | ATOM | 4055 | O   | ALA | A | 510 | 23.176 | 49.243 | 90.747 | 1.00 | 21.57 |
|    | ATOM | 4056 | CB  | ALA | A | 510 | 24.166 | 51.066 | 88.248 | 1.00 | 13.60 |
| 40 | ATOM | 4057 | N   | PRO | A | 511 | 23.755 | 51.340 | 91.417 | 1.00 | 20.55 |
|    | ATOM | 4058 | CA  | PRO | A | 511 | 24.521 | 52.568 | 91.190 | 1.00 | 16.50 |
|    | ATOM | 4059 | C   | PRO | A | 511 | 25.912 | 52.528 | 91.759 | 1.00 | 17.68 |
|    | ATOM | 4060 | O   | PRO | A | 511 | 26.199 | 51.765 | 92.658 | 1.00 | 15.20 |
|    | ATOM | 4061 | CB  | PRO | A | 511 | 23.836 | 53.667 | 92.001 | 1.00 | 15.68 |
| 45 | ATOM | 4062 | CG  | PRO | A | 511 | 23.118 | 52.916 | 93.106 | 1.00 | 22.23 |
|    | ATOM | 4063 | CD  | PRO | A | 511 | 22.859 | 51.497 | 92.597 | 1.00 | 18.77 |
|    | ATOM | 4064 | N   | LEU | A | 512 | 26.755 | 53.380 | 91.203 | 1.00 | 19.26 |
|    | ATOM | 4065 | CA  | LEU | A | 512 | 28.070 | 53.588 | 91.751 | 1.00 | 19.26 |
|    | ATOM | 4066 | C   | LEU | A | 512 | 27.964 | 54.919 | 92.529 | 1.00 | 19.35 |
| 50 | ATOM | 4067 | O   | LEU | A | 512 | 27.053 | 55.732 | 92.316 | 1.00 | 15.40 |
|    | ATOM | 4068 | CB  | LEU | A | 512 | 29.183 | 53.659 | 90.683 | 1.00 | 19.06 |
|    | ATOM | 4069 | CG  | LEU | A | 512 | 29.796 | 52.274 | 90.415 | 1.00 | 23.85 |
|    | ATOM | 4070 | CD1 | LEU | A | 512 | 28.762 | 51.351 | 89.763 | 1.00 | 24.14 |
|    | ATOM | 4071 | CD2 | LEU | A | 512 | 30.975 | 52.408 | 89.453 | 1.00 | 17.31 |
| 55 | ATOM | 4072 | N   | PRO | A | 513 | 28.880 | 55.157 | 93.459 | 1.00 | 18.91 |
|    | ATOM | 4073 | CA  | PRO | A | 513 | 28.823 | 56.408 | 94.168 | 1.00 | 16.34 |
|    | ATOM | 4074 | C   | PRO | A | 513 | 28.925 | 57.520 | 93.140 | 1.00 | 17.64 |
|    | ATOM | 4075 | O   | PRO | A | 513 | 29.686 | 57.443 | 92.192 | 1.00 | 15.39 |
|    | ATOM | 4076 | CB  | PRO | A | 513 | 30.031 | 56.431 | 95.107 | 1.00 | 16.06 |
| 60 | ATOM | 4077 | CG  | PRO | A | 513 | 30.443 | 54.972 | 95.246 | 1.00 | 21.97 |
|    | ATOM | 4078 | CD  | PRO | A | 513 | 29.960 | 54.270 | 93.987 | 1.00 | 17.15 |
|    | ATOM | 4079 | N   | LEU | A | 514 | 28.154 | 58.573 | 93.341 | 1.00 | 19.37 |
|    | ATOM | 4080 | CA  | LEU | A | 514 | 28.155 | 59.712 | 92.431 | 1.00 | 20.71 |
|    | ATOM | 4081 | C   | LEU | A | 514 | 29.567 | 60.240 | 92.151 | 1.00 | 22.73 |
|    | ATOM | 4082 | O   | LEU | A | 514 | 29.934 | 60.486 | 90.991 | 1.00 | 20.91 |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
|    | ATOM | 4083 | CB  | LEU | A | 514 | 27.209 | 60.816 | 92.955 | 1.00 | 19.46 |
|    | ATOM | 4084 | CG  | LEU | A | 514 | 27.173 | 62.058 | 92.077 | 1.00 | 23.47 |
|    | ATOM | 4085 | CD1 | LEU | A | 514 | 26.650 | 61.694 | 90.681 | 1.00 | 21.60 |
| 5  | ATOM | 4086 | CD2 | LEU | A | 514 | 26.275 | 63.087 | 92.767 | 1.00 | 19.09 |
|    | ATOM | 4087 | N   | GLY | A | 515 | 30.353 | 60.384 | 93.236 | 1.00 | 19.02 |
|    | ATOM | 4088 | CA  | GLY | A | 515 | 31.711 | 60.866 | 93.104 | 1.00 | 16.33 |
|    | ATOM | 4089 | C   | GLY | A | 515 | 32.489 | 60.000 | 92.121 | 1.00 | 20.68 |
|    | ATOM | 4090 | O   | GLY | A | 515 | 33.336 | 60.489 | 91.363 | 1.00 | 17.47 |
| 10 | ATOM | 4091 | N   | HIS | A | 516 | 32.199 | 58.691 | 92.105 | 1.00 | 16.69 |
|    | ATOM | 4092 | CA  | HIS | A | 516 | 32.961 | 57.829 | 91.206 | 1.00 | 16.67 |
|    | ATOM | 4093 | C   | HIS | A | 516 | 32.629 | 58.092 | 89.762 | 1.00 | 16.39 |
|    | ATOM | 4094 | O   | HIS | A | 516 | 33.485 | 58.094 | 88.886 | 1.00 | 13.40 |
|    | ATOM | 4095 | CB  | HIS | A | 516 | 32.781 | 56.335 | 91.479 | 1.00 | 16.85 |
| 15 | ATOM | 4096 | CG  | HIS | A | 516 | 33.328 | 55.909 | 92.786 | 1.00 | 23.07 |
|    | ATOM | 4097 | ND1 | HIS | A | 516 | 33.586 | 56.811 | 93.804 | 1.00 | 27.10 |
|    | ATOM | 4098 | CD2 | HIS | A | 516 | 33.691 | 54.664 | 93.219 | 1.00 | 26.55 |
|    | ATOM | 4099 | CE1 | HIS | A | 516 | 34.067 | 56.096 | 94.831 | 1.00 | 27.40 |
|    | ATOM | 4100 | NE2 | HIS | A | 516 | 34.144 | 54.803 | 94.514 | 1.00 | 26.59 |
| 20 | ATOM | 4101 | N   | ILE | A | 517 | 31.349 | 58.288 | 89.534 | 1.00 | 14.76 |
|    | ATOM | 4102 | CA  | ILE | A | 517 | 30.887 | 58.520 | 88.189 | 1.00 | 15.71 |
|    | ATOM | 4103 | C   | ILE | A | 517 | 31.444 | 59.817 | 87.666 | 1.00 | 13.62 |
|    | ATOM | 4104 | O   | ILE | A | 517 | 31.851 | 59.960 | 86.511 | 1.00 | 13.02 |
|    | ATOM | 4105 | CB  | ILE | A | 517 | 29.350 | 58.408 | 88.144 | 1.00 | 20.46 |
| 25 | ATOM | 4106 | CG1 | ILE | A | 517 | 28.925 | 56.989 | 88.555 | 1.00 | 23.97 |
|    | ATOM | 4107 | CG2 | ILE | A | 517 | 28.793 | 58.653 | 86.750 | 1.00 | 19.51 |
|    | ATOM | 4108 | CD1 | ILE | A | 517 | 29.636 | 55.831 | 87.826 | 1.00 | 21.92 |
|    | ATOM | 4109 | N   | LYS | A | 518 | 31.433 | 60.804 | 88.549 | 1.00 | 13.76 |
|    | ATOM | 4110 | CA  | LYS | A | 518 | 32.004 | 62.082 | 88.137 | 1.00 | 12.83 |
| 30 | ATOM | 4111 | C   | LYS | A | 518 | 33.487 | 61.877 | 87.759 | 1.00 | 17.13 |
|    | ATOM | 4112 | O   | LYS | A | 518 | 33.971 | 62.371 | 86.745 | 1.00 | 14.95 |
|    | ATOM | 4113 | CB  | LYS | A | 518 | 31.858 | 63.092 | 89.279 | 1.00 | 12.59 |
|    | ATOM | 4114 | CG  | LYS | A | 518 | 30.392 | 63.447 | 89.416 | 1.00 | 15.77 |
|    | ATOM | 4115 | CD  | LYS | A | 518 | 30.169 | 64.528 | 90.446 | 1.00 | 25.59 |
| 35 | ATOM | 4116 | CE  | LYS | A | 518 | 28.743 | 65.047 | 90.425 | 1.00 | 26.22 |
|    | ATOM | 4117 | NZ  | LYS | A | 518 | 28.669 | 66.440 | 90.886 | 1.00 | 26.75 |
|    | ATOM | 4118 | N   | ARG | A | 519 | 34.237 | 61.144 | 88.604 | 1.00 | 15.99 |
|    | ATOM | 4119 | CA  | ARG | A | 519 | 35.647 | 60.914 | 88.321 | 1.00 | 13.25 |
|    | ATOM | 4120 | C   | ARG | A | 519 | 35.803 | 60.213 | 86.998 | 1.00 | 16.26 |
| 40 | ATOM | 4121 | O   | ARG | A | 519 | 36.679 | 60.478 | 86.216 | 1.00 | 13.50 |
|    | ATOM | 4122 | CB  | ARG | A | 519 | 36.265 | 60.075 | 89.423 | 1.00 | 14.16 |
|    | ATOM | 4123 | CG  | ARG | A | 519 | 37.741 | 59.741 | 89.216 | 1.00 | 13.79 |
|    | ATOM | 4124 | CD  | ARG | A | 519 | 38.685 | 60.955 | 89.134 | 1.00 | 22.42 |
|    | ATOM | 4125 | NE  | ARG | A | 519 | 40.127 | 60.613 | 89.069 | 1.00 | 17.77 |
| 45 | ATOM | 4126 | CZ  | ARG | A | 519 | 41.035 | 61.432 | 88.570 | 1.00 | 19.26 |
|    | ATOM | 4127 | NH1 | ARG | A | 519 | 40.692 | 62.640 | 88.087 | 1.00 | 18.57 |
|    | ATOM | 4128 | NH2 | ARG | A | 519 | 42.289 | 61.014 | 88.549 | 1.00 | 17.51 |
|    | ATOM | 4129 | N   | MET | A | 520 | 34.897 | 59.292 | 86.743 | 1.00 | 13.85 |
|    | ATOM | 4130 | CA  | MET | A | 520 | 34.944 | 58.548 | 85.514 | 1.00 | 13.32 |
| 50 | ATOM | 4131 | C   | MET | A | 520 | 34.803 | 59.460 | 84.299 | 1.00 | 16.61 |
|    | ATOM | 4132 | O   | MET | A | 520 | 35.461 | 59.286 | 83.279 | 1.00 | 15.39 |
|    | ATOM | 4133 | CB  | MET | A | 520 | 33.860 | 57.425 | 85.585 | 1.00 | 15.92 |
|    | ATOM | 4134 | CG  | MET | A | 520 | 33.887 | 56.502 | 84.369 | 1.00 | 16.73 |
|    | ATOM | 4135 | SD  | MET | A | 520 | 32.699 | 55.131 | 84.463 | 1.00 | 19.40 |
| 55 | ATOM | 4136 | CE  | MET | A | 520 | 33.250 | 54.267 | 85.942 | 1.00 | 17.31 |
|    | ATOM | 4137 | N   | GLN | A | 521 | 33.919 | 60.449 | 84.358 | 1.00 | 10.96 |
|    | ATOM | 4138 | CA  | GLN | A | 521 | 33.800 | 61.336 | 83.205 | 1.00 | 10.25 |
|    | ATOM | 4139 | C   | GLN | A | 521 | 35.105 | 62.160 | 83.122 | 1.00 | 14.21 |
|    | ATOM | 4140 | O   | GLN | A | 521 | 35.684 | 62.487 | 82.073 | 1.00 | 11.43 |
| 60 | ATOM | 4141 | CB  | GLN | A | 521 | 32.548 | 62.237 | 83.376 | 1.00 | 9.22  |
|    | ATOM | 4142 | CG  | GLN | A | 521 | 32.547 | 63.519 | 82.503 | 1.00 | 12.68 |
|    | ATOM | 4143 | CD  | GLN | A | 521 | 32.758 | 63.301 | 81.025 | 1.00 | 18.23 |
|    | ATOM | 4144 | OE1 | GLN | A | 521 | 33.271 | 64.187 | 80.309 | 1.00 | 20.20 |
|    | ATOM | 4145 | NE2 | GLN | A | 521 | 32.453 | 62.102 | 80.554 | 1.00 | 10.43 |
|    | ATOM | 4146 | N   | GLU | A | 522 | 35.608 | 62.524 | 84.295 | 1.00 | 15.29 |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
|    | ATOM | 4147 | CA  | GLU | A | 522 | 36.816 | 63.335 | 84.345 | 1.00 | 14.86 |
|    | ATOM | 4148 | C   | GLU | A | 522 | 38.026 | 62.632 | 83.702 | 1.00 | 24.87 |
|    | ATOM | 4149 | O   | GLU | A | 522 | 38.848 | 63.232 | 82.990 | 1.00 | 19.95 |
| 5  | ATOM | 4150 | CB  | GLU | A | 522 | 37.068 | 63.573 | 85.820 | 1.00 | 15.93 |
|    | ATOM | 4151 | CG  | GLU | A | 522 | 38.175 | 64.573 | 86.121 | 1.00 | 34.79 |
|    | ATOM | 4152 | CD  | GLU | A | 522 | 38.013 | 64.959 | 87.556 | 1.00 | 61.54 |
|    | ATOM | 4153 | OE1 | GLU | A | 522 | 38.436 | 64.271 | 88.466 | 1.00 | 24.02 |
|    | ATOM | 4154 | OE2 | GLU | A | 522 | 37.252 | 66.014 | 87.710 | 1.00 | 60.58 |
| 10 | ATOM | 4155 | N   | VAL | A | 523 | 38.179 | 61.338 | 83.966 | 1.00 | 17.81 |
|    | ATOM | 4156 | CA  | VAL | A | 523 | 39.302 | 60.635 | 83.392 | 1.00 | 17.49 |
|    | ATOM | 4157 | C   | VAL | A | 523 | 39.081 | 60.051 | 81.994 | 1.00 | 17.20 |
|    | ATOM | 4158 | O   | VAL | A | 523 | 40.038 | 59.940 | 81.230 | 1.00 | 22.12 |
|    | ATOM | 4159 | CB  | VAL | A | 523 | 39.952 | 59.621 | 84.340 | 1.00 | 18.80 |
| 15 | ATOM | 4160 | CG1 | VAL | A | 523 | 40.427 | 60.324 | 85.613 | 1.00 | 18.67 |
|    | ATOM | 4161 | CG2 | VAL | A | 523 | 38.957 | 58.522 | 84.717 | 1.00 | 17.30 |
|    | ATOM | 4162 | N   | TYR | A | 524 | 37.851 | 59.676 | 81.633 | 1.00 | 13.33 |
|    | ATOM | 4163 | CA  | TYR | A | 524 | 37.638 | 59.045 | 80.331 | 1.00 | 12.09 |
|    | ATOM | 4164 | C   | TYR | A | 524 | 36.842 | 59.839 | 79.321 | 1.00 | 19.77 |
| 20 | ATOM | 4165 | O   | TYR | A | 524 | 36.720 | 59.417 | 78.179 | 1.00 | 17.94 |
|    | ATOM | 4166 | CB  | TYR | A | 524 | 36.961 | 57.656 | 80.463 | 1.00 | 13.83 |
|    | ATOM | 4167 | CG  | TYR | A | 524 | 37.615 | 56.667 | 81.421 | 1.00 | 14.86 |
|    | ATOM | 4168 | CD1 | TYR | A | 524 | 38.999 | 56.608 | 81.574 | 1.00 | 13.07 |
|    | ATOM | 4169 | CD2 | TYR | A | 524 | 36.832 | 55.761 | 82.146 | 1.00 | 19.57 |
| 25 | ATOM | 4170 | CE1 | TYR | A | 524 | 39.592 | 55.704 | 82.460 | 1.00 | 18.13 |
|    | ATOM | 4171 | CE2 | TYR | A | 524 | 37.403 | 54.832 | 83.019 | 1.00 | 18.46 |
|    | ATOM | 4172 | CZ  | TYR | A | 524 | 38.790 | 54.813 | 83.181 | 1.00 | 17.58 |
|    | ATOM | 4173 | OH  | TYR | A | 524 | 39.360 | 53.937 | 84.087 | 1.00 | 16.81 |
|    | ATOM | 4174 | N   | ASN | A | 525 | 36.235 | 60.940 | 79.753 | 1.00 | 20.91 |
| 30 | ATOM | 4175 | CA  | ASN | A | 525 | 35.435 | 61.755 | 78.865 | 1.00 | 16.88 |
|    | ATOM | 4176 | C   | ASN | A | 525 | 34.488 | 60.923 | 78.018 | 1.00 | 18.05 |
|    | ATOM | 4177 | O   | ASN | A | 525 | 34.450 | 61.014 | 76.789 | 1.00 | 15.92 |
|    | ATOM | 4178 | CB  | ASN | A | 525 | 36.361 | 62.615 | 78.002 | 1.00 | 13.81 |
|    | ATOM | 4179 | CG  | ASN | A | 525 | 35.680 | 63.751 | 77.259 | 1.00 | 18.94 |
| 35 | ATOM | 4180 | OD1 | ASN | A | 525 | 36.243 | 64.268 | 76.280 | 1.00 | 18.98 |
|    | ATOM | 4181 | ND2 | ASN | A | 525 | 34.502 | 64.169 | 77.693 | 1.00 | 14.31 |
|    | ATOM | 4182 | N   | PHE | A | 526 | 33.659 | 60.120 | 78.683 | 1.00 | 14.70 |
|    | ATOM | 4183 | CA  | PHE | A | 526 | 32.676 | 59.337 | 77.947 | 1.00 | 12.71 |
|    | ATOM | 4184 | C   | PHE | A | 526 | 31.596 | 60.234 | 77.380 | 1.00 | 16.60 |
| 40 | ATOM | 4185 | O   | PHE | A | 526 | 30.891 | 59.866 | 76.439 | 1.00 | 15.88 |
|    | ATOM | 4186 | CB  | PHE | A | 526 | 32.038 | 58.303 | 78.876 | 1.00 | 14.35 |
|    | ATOM | 4187 | CG  | PHE | A | 526 | 32.957 | 57.130 | 79.130 | 1.00 | 15.85 |
|    | ATOM | 4188 | CD1 | PHE | A | 526 | 33.895 | 56.735 | 78.175 | 1.00 | 19.68 |
|    | ATOM | 4189 | CD2 | PHE | A | 526 | 32.876 | 56.397 | 80.314 | 1.00 | 16.85 |
| 45 | ATOM | 4190 | CE1 | PHE | A | 526 | 34.687 | 55.604 | 78.378 | 1.00 | 21.64 |
|    | ATOM | 4191 | CE2 | PHE | A | 526 | 33.698 | 55.298 | 80.567 | 1.00 | 19.90 |
|    | ATOM | 4192 | CZ  | PHE | A | 526 | 34.590 | 54.890 | 79.575 | 1.00 | 18.31 |
|    | ATOM | 4193 | N   | ASN | A | 527 | 31.418 | 61.433 | 77.949 | 1.00 | 12.75 |
|    | ATOM | 4194 | CA  | ASN | A | 527 | 30.391 | 62.355 | 77.446 | 1.00 | 12.28 |
| 50 | ATOM | 4195 | C   | ASN | A | 527 | 30.627 | 62.668 | 75.971 | 1.00 | 19.85 |
|    | ATOM | 4196 | O   | ASN | A | 527 | 29.715 | 62.907 | 75.185 | 1.00 | 18.13 |
|    | ATOM | 4197 | CB  | ASN | A | 527 | 30.431 | 63.713 | 78.160 | 1.00 | 13.86 |
|    | ATOM | 4198 | CG  | ASN | A | 527 | 29.641 | 63.696 | 79.434 | 1.00 | 25.14 |
|    | ATOM | 4199 | OD1 | ASN | A | 527 | 29.760 | 64.600 | 80.250 | 1.00 | 20.32 |
| 55 | ATOM | 4200 | ND2 | ASN | A | 527 | 28.830 | 62.668 | 79.610 | 1.00 | 10.82 |
|    | ATOM | 4201 | N   | ALA | A | 528 | 31.906 | 62.668 | 75.607 | 1.00 | 15.34 |
|    | ATOM | 4202 | CA  | ALA | A | 528 | 32.280 | 62.964 | 74.264 | 1.00 | 17.72 |
|    | ATOM | 4203 | C   | ALA | A | 528 | 32.075 | 61.861 | 73.228 | 1.00 | 26.48 |
|    | ATOM | 4204 | O   | ALA | A | 528 | 32.198 | 62.127 | 72.031 | 1.00 | 21.26 |
| 60 | ATOM | 4205 | CB  | ALA | A | 528 | 33.729 | 63.372 | 74.236 | 1.00 | 18.38 |
|    | ATOM | 4206 | N   | ILE | A | 529 | 31.810 | 60.629 | 73.664 | 1.00 | 19.00 |
|    | ATOM | 4207 | CA  | ILE | A | 529 | 31.690 | 59.524 | 72.731 | 1.00 | 15.58 |
|    | ATOM | 4208 | C   | ILE | A | 529 | 30.389 | 59.499 | 71.945 | 1.00 | 15.90 |
|    | ATOM | 4209 | O   | ILE | A | 529 | 29.305 | 59.561 | 72.494 | 1.00 | 16.45 |
|    | ATOM | 4210 | CB  | ILE | A | 529 | 31.946 | 58.208 | 73.454 | 1.00 | 17.38 |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
|    | ATOM | 4211 | CG1 | ILE | A | 529 | 33.456 | 58.159 | 73.709 | 1.00 | 19.42 |
|    | ATOM | 4212 | CG2 | ILE | A | 529 | 31.511 | 57.103 | 72.488 | 1.00 | 17.67 |
|    | ATOM | 4213 | CD1 | ILE | A | 529 | 34.027 | 57.047 | 74.576 | 1.00 | 23.37 |
| 5  | ATOM | 4214 | N   | ASN | A | 530 | 30.440 | 59.418 | 70.641 | 1.00 | 16.94 |
|    | ATOM | 4215 | CA  | ASN | A | 530 | 29.151 | 59.417 | 69.969 | 1.00 | 20.74 |
|    | ATOM | 4216 | C   | ASN | A | 530 | 28.522 | 58.081 | 69.611 | 1.00 | 25.19 |
|    | ATOM | 4217 | O   | ASN | A | 530 | 27.369 | 58.026 | 69.217 | 1.00 | 23.63 |
|    | ATOM | 4218 | CB  | ASN | A | 530 | 28.937 | 60.566 | 68.986 | 1.00 | 39.14 |
| 10 | ATOM | 4219 | CG  | ASN | A | 530 | 28.612 | 61.852 | 69.749 | 1.00 | 80.92 |
|    | ATOM | 4220 | OD1 | ASN | A | 530 | 27.639 | 61.959 | 70.533 | 1.00 | 86.83 |
|    | ATOM | 4221 | ND2 | ASN | A | 530 | 29.470 | 62.838 | 69.537 | 1.00 | 45.14 |
|    | ATOM | 4222 | N   | ASN | A | 531 | 29.306 | 57.019 | 69.759 | 1.00 | 19.99 |
|    | ATOM | 4223 | CA  | ASN | A | 531 | 28.875 | 55.667 | 69.494 | 1.00 | 18.88 |
| 15 | ATOM | 4224 | C   | ASN | A | 531 | 27.637 | 55.452 | 70.350 | 1.00 | 15.67 |
|    | ATOM | 4225 | O   | ASN | A | 531 | 27.671 | 55.661 | 71.566 | 1.00 | 15.13 |
|    | ATOM | 4226 | CB  | ASN | A | 531 | 30.045 | 54.762 | 69.928 | 1.00 | 11.62 |
|    | ATOM | 4227 | CG  | ASN | A | 531 | 29.705 | 53.292 | 69.866 | 1.00 | 26.73 |
|    | ATOM | 4228 | OD1 | ASN | A | 531 | 28.724 | 52.832 | 70.471 | 1.00 | 21.97 |
| 20 | ATOM | 4229 | ND2 | ASN | A | 531 | 30.510 | 52.554 | 69.105 | 1.00 | 18.28 |
|    | ATOM | 4230 | N   | SER | A | 532 | 26.551 | 55.074 | 69.715 | 1.00 | 12.93 |
|    | ATOM | 4231 | CA  | SER | A | 532 | 25.293 | 54.931 | 70.456 | 1.00 | 15.99 |
|    | ATOM | 4232 | C   | SER | A | 532 | 25.248 | 53.889 | 71.565 | 1.00 | 17.50 |
|    | ATOM | 4233 | O   | SER | A | 532 | 24.631 | 54.066 | 72.611 | 1.00 | 20.47 |
| 25 | ATOM | 4234 | CB  | SER | A | 532 | 24.088 | 54.846 | 69.518 | 1.00 | 17.43 |
|    | ATOM | 4235 | OG  | SER | A | 532 | 24.274 | 53.791 | 68.570 | 1.00 | 24.83 |
|    | ATOM | 4236 | N   | GLU | A | 533 | 25.876 | 52.753 | 71.337 | 1.00 | 14.65 |
|    | ATOM | 4237 | CA  | GLU | A | 533 | 25.835 | 51.708 | 72.339 | 1.00 | 13.13 |
|    | ATOM | 4238 | C   | GLU | A | 533 | 26.497 | 52.181 | 73.614 | 1.00 | 19.42 |
| 30 | ATOM | 4239 | O   | GLU | A | 533 | 25.964 | 52.028 | 74.725 | 1.00 | 15.25 |
|    | ATOM | 4240 | CB  | GLU | A | 533 | 26.547 | 50.464 | 71.780 | 1.00 | 13.22 |
|    | ATOM | 4241 | CG  | GLU | A | 533 | 25.712 | 49.829 | 70.637 | 1.00 | 9.87  |
|    | ATOM | 4242 | CD  | GLU | A | 533 | 24.531 | 49.055 | 71.162 | 1.00 | 21.99 |
|    | ATOM | 4243 | OE1 | GLU | A | 533 | 24.395 | 48.722 | 72.319 | 1.00 | 18.49 |
| 35 | ATOM | 4244 | OE2 | GLU | A | 533 | 23.625 | 48.805 | 70.267 | 1.00 | 16.24 |
|    | ATOM | 4245 | N   | ILE | A | 534 | 27.686 | 52.747 | 73.415 | 1.00 | 15.22 |
|    | ATOM | 4246 | CA  | ILE | A | 534 | 28.495 | 53.265 | 74.512 | 1.00 | 14.94 |
|    | ATOM | 4247 | C   | ILE | A | 534 | 27.793 | 54.420 | 75.228 | 1.00 | 14.04 |
|    | ATOM | 4248 | O   | ILE | A | 534 | 27.677 | 54.447 | 76.461 | 1.00 | 17.42 |
| 40 | ATOM | 4249 | CB  | ILE | A | 534 | 29.926 | 53.655 | 74.077 | 1.00 | 17.98 |
|    | ATOM | 4250 | CG1 | ILE | A | 534 | 30.733 | 52.461 | 73.557 | 1.00 | 13.41 |
|    | ATOM | 4251 | CG2 | ILE | A | 534 | 30.680 | 54.387 | 75.216 | 1.00 | 15.34 |
|    | ATOM | 4252 | CD1 | ILE | A | 534 | 32.003 | 52.906 | 72.825 | 1.00 | 17.39 |
|    | ATOM | 4253 | N   | ARG | A | 535 | 27.310 | 55.402 | 74.475 | 1.00 | 14.39 |
| 45 | ATOM | 4254 | CA  | ARG | A | 535 | 26.611 | 56.511 | 75.135 | 1.00 | 17.35 |
|    | ATOM | 4255 | C   | ARG | A | 535 | 25.347 | 56.016 | 75.868 | 1.00 | 14.54 |
|    | ATOM | 4256 | O   | ARG | A | 535 | 24.998 | 56.382 | 76.973 | 1.00 | 15.05 |
|    | ATOM | 4257 | CB  | ARG | A | 535 | 26.232 | 57.576 | 74.108 | 1.00 | 16.26 |
|    | ATOM | 4258 | CG  | ARG | A | 535 | 25.583 | 58.826 | 74.730 | 1.00 | 8.73  |
| 50 | ATOM | 4259 | CD  | ARG | A | 535 | 25.392 | 59.919 | 73.666 | 1.00 | 11.55 |
|    | ATOM | 4260 | NE  | ARG | A | 535 | 25.126 | 61.228 | 74.251 | 1.00 | 15.18 |
|    | ATOM | 4261 | CZ  | ARG | A | 535 | 26.049 | 62.043 | 74.761 | 1.00 | 26.20 |
|    | ATOM | 4262 | NH1 | ARG | A | 535 | 27.354 | 61.765 | 74.769 | 1.00 | 20.26 |
|    | ATOM | 4263 | NH2 | ARG | A | 535 | 25.636 | 63.189 | 75.286 | 1.00 | 19.91 |
| 55 | ATOM | 4264 | N   | PHE | A | 536 | 24.632 | 55.126 | 75.233 | 1.00 | 11.71 |
|    | ATOM | 4265 | CA  | PHE | A | 536 | 23.462 | 54.627 | 75.876 | 1.00 | 9.63  |
|    | ATOM | 4266 | C   | PHE | A | 536 | 23.825 | 54.092 | 77.233 | 1.00 | 13.77 |
|    | ATOM | 4267 | O   | PHE | A | 536 | 23.256 | 54.497 | 78.231 | 1.00 | 13.81 |
|    | ATOM | 4268 | CB  | PHE | A | 536 | 22.906 | 53.471 | 75.016 | 1.00 | 10.66 |
| 60 | ATOM | 4269 | CG  | PHE | A | 536 | 21.865 | 52.621 | 75.710 | 1.00 | 14.64 |
|    | ATOM | 4270 | CD1 | PHE | A | 536 | 20.699 | 53.158 | 76.256 | 1.00 | 13.81 |
|    | ATOM | 4271 | CD2 | PHE | A | 536 | 22.052 | 51.242 | 75.840 | 1.00 | 19.23 |
|    | ATOM | 4272 | CE1 | PHE | A | 536 | 19.762 | 52.325 | 76.877 | 1.00 | 14.23 |
|    | ATOM | 4273 | CE2 | PHE | A | 536 | 21.127 | 50.395 | 76.457 | 1.00 | 16.53 |
|    | ATOM | 4274 | CZ  | PHE | A | 536 | 19.960 | 50.945 | 76.984 | 1.00 | 11.63 |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
|    | ATOM | 4275 | N   | ARG | A | 537 | 24.750 | 53.131 | 77.282 | 1.00 | 12.89 |
|    | ATOM | 4276 | CA  | ARG | A | 537 | 25.110 | 52.536 | 78.577 | 1.00 | 11.92 |
|    | ATOM | 4277 | C   | ARG | A | 537 | 25.734 | 53.520 | 79.575 | 1.00 | 16.03 |
| 5  | ATOM | 4278 | O   | ARG | A | 537 | 25.525 | 53.436 | 80.793 | 1.00 | 10.71 |
|    | ATOM | 4279 | CB  | ARG | A | 537 | 25.949 | 51.253 | 78.505 | 1.00 | 11.85 |
|    | ATOM | 4280 | CG  | ARG | A | 537 | 25.274 | 50.113 | 77.776 | 1.00 | 8.59  |
|    | ATOM | 4281 | CD  | ARG | A | 537 | 26.142 | 48.857 | 77.547 | 1.00 | 17.16 |
|    | ATOM | 4282 | NE  | ARG | A | 537 | 25.233 | 47.845 | 76.992 | 1.00 | 16.12 |
| 10 | ATOM | 4283 | CZ  | ARG | A | 537 | 24.869 | 47.824 | 75.716 | 1.00 | 25.23 |
|    | ATOM | 4284 | NH1 | ARG | A | 537 | 25.414 | 48.641 | 74.802 | 1.00 | 13.55 |
|    | ATOM | 4285 | NH2 | ARG | A | 537 | 23.946 | 46.947 | 75.356 | 1.00 | 16.52 |
|    | ATOM | 4286 | N   | TRP | A | 538 | 26.544 | 54.451 | 79.060 | 1.00 | 13.16 |
|    | ATOM | 4287 | CA  | TRP | A | 538 | 27.170 | 55.440 | 79.907 | 1.00 | 10.77 |
| 15 | ATOM | 4288 | C   | TRP | A | 538 | 26.079 | 56.286 | 80.532 | 1.00 | 13.43 |
|    | ATOM | 4289 | O   | TRP | A | 538 | 26.048 | 56.509 | 81.736 | 1.00 | 13.45 |
|    | ATOM | 4290 | CB  | TRP | A | 538 | 28.036 | 56.318 | 78.996 | 1.00 | 12.97 |
|    | ATOM | 4291 | CG  | TRP | A | 538 | 28.489 | 57.611 | 79.604 | 1.00 | 12.46 |
|    | ATOM | 4292 | CD1 | TRP | A | 538 | 28.330 | 58.807 | 79.019 | 1.00 | 13.56 |
| 20 | ATOM | 4293 | CD2 | TRP | A | 538 | 29.199 | 57.826 | 80.857 | 1.00 | 11.95 |
|    | ATOM | 4294 | NE1 | TRP | A | 538 | 28.932 | 59.757 | 79.801 | 1.00 | 12.84 |
|    | ATOM | 4295 | CE2 | TRP | A | 538 | 29.455 | 59.208 | 80.938 | 1.00 | 12.68 |
|    | ATOM | 4296 | CE3 | TRP | A | 538 | 29.667 | 57.000 | 81.914 | 1.00 | 11.87 |
|    | ATOM | 4297 | CZ2 | TRP | A | 538 | 30.115 | 59.780 | 82.024 | 1.00 | 10.55 |
|    | ATOM | 4298 | CZ3 | TRP | A | 538 | 30.334 | 57.557 | 82.994 | 1.00 | 12.97 |
| 25 | ATOM | 4299 | CH2 | TRP | A | 538 | 30.537 | 58.953 | 83.046 | 1.00 | 14.62 |
|    | ATOM | 4300 | N   | LEU | A | 539 | 25.160 | 56.761 | 79.714 | 1.00 | 8.88  |
|    | ATOM | 4301 | CA  | LEU | A | 539 | 24.132 | 57.592 | 80.310 | 1.00 | 11.52 |
|    | ATOM | 4302 | C   | LEU | A | 539 | 23.249 | 56.878 | 81.335 | 1.00 | 17.64 |
| 30 | ATOM | 4303 | O   | LEU | A | 539 | 22.775 | 57.470 | 82.308 | 1.00 | 15.29 |
|    | ATOM | 4304 | CB  | LEU | A | 539 | 23.253 | 58.271 | 79.251 | 1.00 | 13.68 |
|    | ATOM | 4305 | CG  | LEU | A | 539 | 23.977 | 59.247 | 78.323 | 1.00 | 15.24 |
|    | ATOM | 4306 | CD1 | LEU | A | 539 | 22.989 | 59.923 | 77.388 | 1.00 | 13.27 |
|    | ATOM | 4307 | CD2 | LEU | A | 539 | 24.693 | 60.312 | 79.121 | 1.00 | 13.80 |
| 35 | ATOM | 4308 | N   | ARG | A | 540 | 22.988 | 55.583 | 81.115 | 1.00 | 14.05 |
|    | ATOM | 4309 | CA  | ARG | A | 540 | 22.176 | 54.850 | 82.067 | 1.00 | 11.62 |
|    | ATOM | 4310 | C   | ARG | A | 540 | 22.880 | 54.792 | 83.418 | 1.00 | 13.27 |
|    | ATOM | 4311 | O   | ARG | A | 540 | 22.277 | 54.942 | 84.488 | 1.00 | 12.86 |
|    | ATOM | 4312 | CB  | ARG | A | 540 | 21.883 | 53.426 | 81.584 | 1.00 | 12.88 |
| 40 | ATOM | 4313 | CG  | ARG | A | 540 | 20.894 | 53.325 | 80.408 | 1.00 | 8.76  |
|    | ATOM | 4314 | CD  | ARG | A | 540 | 20.453 | 51.857 | 80.281 | 1.00 | 14.08 |
|    | ATOM | 4315 | NE  | ARG | A | 540 | 19.442 | 51.552 | 81.288 | 1.00 | 11.93 |
|    | ATOM | 4316 | CZ  | ARG | A | 540 | 18.856 | 50.391 | 81.486 | 1.00 | 16.72 |
|    | ATOM | 4317 | NH1 | ARG | A | 540 | 19.145 | 49.317 | 80.774 | 1.00 | 16.31 |
|    | ATOM | 4318 | NH2 | ARG | A | 540 | 17.926 | 50.330 | 82.416 | 1.00 | 9.86  |
| 45 | ATOM | 4319 | N   | LEU | A | 541 | 24.189 | 54.546 | 83.338 | 1.00 | 10.69 |
|    | ATOM | 4320 | CA  | LEU | A | 541 | 25.036 | 54.432 | 84.526 | 1.00 | 9.89  |
|    | ATOM | 4321 | C   | LEU | A | 541 | 25.017 | 55.712 | 85.353 | 1.00 | 12.38 |
|    | ATOM | 4322 | O   | LEU | A | 541 | 24.961 | 55.749 | 86.598 | 1.00 | 12.85 |
| 50 | ATOM | 4323 | CB  | LEU | A | 541 | 26.482 | 54.119 | 84.074 | 1.00 | 8.98  |
|    | ATOM | 4324 | CG  | LEU | A | 541 | 27.519 | 53.986 | 85.194 | 1.00 | 13.06 |
|    | ATOM | 4325 | CD1 | LEU | A | 541 | 27.144 | 52.889 | 86.196 | 1.00 | 11.30 |
|    | ATOM | 4326 | CD2 | LEU | A | 541 | 28.904 | 53.697 | 84.606 | 1.00 | 11.15 |
|    | ATOM | 4327 | N   | CYS | A | 542 | 25.097 | 56.800 | 84.603 | 1.00 | 14.91 |
| 55 | ATOM | 4328 | CA  | CYS | A | 542 | 25.043 | 58.147 | 85.153 | 1.00 | 15.42 |
|    | ATOM | 4329 | C   | CYS | A | 542 | 23.719 | 58.436 | 85.881 | 1.00 | 12.87 |
|    | ATOM | 4330 | O   | CYS | A | 542 | 23.689 | 58.913 | 87.019 | 1.00 | 13.42 |
|    | ATOM | 4331 | CB  | CYS | A | 542 | 25.234 | 59.166 | 83.987 | 1.00 | 14.29 |
|    | ATOM | 4332 | SG  | CYS | A | 542 | 26.987 | 59.258 | 83.516 | 1.00 | 15.48 |
| 60 | ATOM | 4333 | N   | ILE | A | 543 | 22.620 | 58.161 | 85.188 | 1.00 | 11.12 |
|    | ATOM | 4334 | CA  | ILE | A | 543 | 21.287 | 58.388 | 85.723 | 1.00 | 12.92 |
|    | ATOM | 4335 | C   | ILE | A | 543 | 21.034 | 57.514 | 86.912 | 1.00 | 15.64 |
|    | ATOM | 4336 | O   | ILE | A | 543 | 20.565 | 57.959 | 87.965 | 1.00 | 14.40 |
|    | ATOM | 4337 | CB  | ILE | A | 543 | 20.193 | 58.168 | 84.670 | 1.00 | 14.69 |
|    | ATOM | 4338 | CG1 | ILE | A | 543 | 20.350 | 59.208 | 83.580 | 1.00 | 14.31 |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
|    | ATOM | 4339 | CG2 | ILE | A | 543 | 18.785 | 58.292 | 85.281 | 1.00 | 11.05 |
|    | ATOM | 4340 | CD1 | ILE | A | 543 | 20.139 | 60.651 | 84.095 | 1.00 | 13.56 |
|    | ATOM | 4341 | N   | GLN | A | 544 | 21.362 | 56.237 | 86.729 | 1.00 | 13.09 |
| 5  | ATOM | 4342 | CA  | GLN | A | 544 | 21.144 | 55.310 | 87.829 | 1.00 | 12.90 |
|    | ATOM | 4343 | C   | GLN | A | 544 | 22.017 | 55.629 | 89.015 | 1.00 | 16.30 |
|    | ATOM | 4344 | O   | GLN | A | 544 | 21.649 | 55.299 | 90.140 | 1.00 | 12.81 |
|    | ATOM | 4345 | CB  | GLN | A | 544 | 21.287 | 53.846 | 87.396 | 1.00 | 14.77 |
|    | ATOM | 4346 | CG  | GLN | A | 544 | 20.159 | 53.374 | 86.449 | 1.00 | 13.43 |
| 10 | ATOM | 4347 | CD  | GLN | A | 544 | 20.399 | 51.967 | 85.889 | 1.00 | 16.60 |
|    | ATOM | 4348 | OE1 | GLN | A | 544 | 20.048 | 51.639 | 84.754 | 1.00 | 18.63 |
|    | ATOM | 4349 | NE2 | GLN | A | 544 | 20.976 | 51.100 | 86.695 | 1.00 | 7.00  |
|    | ATOM | 4350 | N   | SER | A | 545 | 23.143 | 56.296 | 88.748 | 1.00 | 13.80 |
|    | ATOM | 4351 | CA  | SER | A | 545 | 24.058 | 56.712 | 89.799 | 1.00 | 13.01 |
| 15 | ATOM | 4352 | C   | SER | A | 545 | 23.715 | 58.091 | 90.368 | 1.00 | 17.51 |
|    | ATOM | 4353 | O   | SER | A | 545 | 24.429 | 58.656 | 91.189 | 1.00 | 17.76 |
|    | ATOM | 4354 | CB  | SER | A | 545 | 25.495 | 56.649 | 89.330 | 1.00 | 14.26 |
|    | ATOM | 4355 | OG  | SER | A | 545 | 25.735 | 55.273 | 89.138 | 1.00 | 15.74 |
|    | ATOM | 4356 | N   | LYS | A | 546 | 22.586 | 58.609 | 89.924 | 1.00 | 13.25 |
| 20 | ATOM | 4357 | CA  | LYS | A | 546 | 22.029 | 59.857 | 90.370 | 1.00 | 14.37 |
|    | ATOM | 4358 | C   | LYS | A | 546 | 22.771 | 61.109 | 89.963 | 1.00 | 16.71 |
|    | ATOM | 4359 | O   | LYS | A | 546 | 22.770 | 62.106 | 90.698 | 1.00 | 16.30 |
|    | ATOM | 4360 | CB  | LYS | A | 546 | 21.850 | 59.890 | 91.878 | 1.00 | 15.93 |
|    | ATOM | 4361 | CG  | LYS | A | 546 | 21.320 | 58.602 | 92.470 | 1.00 | 16.80 |
| 25 | ATOM | 4362 | CD  | LYS | A | 546 | 19.919 | 58.370 | 91.982 | 1.00 | 13.30 |
|    | ATOM | 4363 | CE  | LYS | A | 546 | 19.280 | 57.148 | 92.617 | 1.00 | 24.82 |
|    | ATOM | 4364 | NZ  | LYS | A | 546 | 18.052 | 56.742 | 91.905 | 1.00 | 17.92 |
|    | ATOM | 4365 | N   | TRP | A | 547 | 23.418 | 61.104 | 88.827 | 1.00 | 15.72 |
|    | ATOM | 4366 | CA  | TRP | A | 547 | 24.103 | 62.319 | 88.438 | 1.00 | 16.24 |
| 30 | ATOM | 4367 | C   | TRP | A | 547 | 23.132 | 63.246 | 87.727 | 1.00 | 18.78 |
|    | ATOM | 4368 | O   | TRP | A | 547 | 22.760 | 63.007 | 86.605 | 1.00 | 16.35 |
|    | ATOM | 4369 | CB  | TRP | A | 547 | 25.261 | 61.999 | 87.505 | 1.00 | 15.42 |
|    | ATOM | 4370 | CG  | TRP | A | 547 | 26.211 | 63.156 | 87.344 | 1.00 | 16.84 |
|    | ATOM | 4371 | CD1 | TRP | A | 547 | 26.177 | 64.386 | 87.949 | 1.00 | 18.62 |
| 35 | ATOM | 4372 | CD2 | TRP | A | 547 | 27.349 | 63.140 | 86.479 | 1.00 | 15.94 |
|    | ATOM | 4373 | NE1 | TRP | A | 547 | 27.267 | 65.115 | 87.543 | 1.00 | 16.22 |
|    | ATOM | 4374 | CE2 | TRP | A | 547 | 27.997 | 64.380 | 86.629 | 1.00 | 18.06 |
|    | ATOM | 4375 | CE3 | TRP | A | 547 | 27.900 | 62.159 | 85.647 | 1.00 | 16.57 |
|    | ATOM | 4376 | CZ2 | TRP | A | 547 | 29.186 | 64.662 | 85.928 | 1.00 | 16.68 |
| 40 | ATOM | 4377 | CZ3 | TRP | A | 547 | 29.068 | 62.459 | 84.966 | 1.00 | 19.03 |
|    | ATOM | 4378 | CH2 | TRP | A | 547 | 29.693 | 63.709 | 85.079 | 1.00 | 18.04 |
|    | ATOM | 4379 | N   | GLU | A | 548 | 22.706 | 64.327 | 88.376 | 1.00 | 13.95 |
|    | ATOM | 4380 | CA  | GLU | A | 548 | 21.745 | 65.238 | 87.780 | 1.00 | 13.21 |
|    | ATOM | 4381 | C   | GLU | A | 548 | 22.176 | 65.856 | 86.468 | 1.00 | 17.27 |
| 45 | ATOM | 4382 | O   | GLU | A | 548 | 21.352 | 66.149 | 85.617 | 1.00 | 18.18 |
|    | ATOM | 4383 | CB  | GLU | A | 548 | 21.375 | 66.370 | 88.771 | 1.00 | 15.29 |
|    | ATOM | 4384 | CG  | GLU | A | 548 | 20.751 | 65.878 | 90.109 | 1.00 | 19.42 |
|    | ATOM | 4385 | CD  | GLU | A | 548 | 20.207 | 67.018 | 90.953 | 1.00 | 33.00 |
|    | ATOM | 4386 | OE1 | GLU | A | 548 | 19.775 | 68.057 | 90.492 | 1.00 | 46.88 |
| 50 | ATOM | 4387 | OE2 | GLU | A | 548 | 20.224 | 66.791 | 92.239 | 1.00 | 30.89 |
|    | ATOM | 4388 | N   | ASP | A | 549 | 23.477 | 66.105 | 86.285 | 1.00 | 17.99 |
|    | ATOM | 4389 | CA  | ASP | A | 549 | 23.929 | 66.735 | 85.054 | 1.00 | 10.58 |
|    | ATOM | 4390 | C   | ASP | A | 549 | 23.666 | 65.896 | 83.853 | 1.00 | 12.02 |
|    | ATOM | 4391 | O   | ASP | A | 549 | 23.629 | 66.354 | 82.709 | 1.00 | 18.87 |
| 55 | ATOM | 4392 | CB  | ASP | A | 549 | 25.426 | 67.034 | 85.126 | 1.00 | 11.36 |
|    | ATOM | 4393 | CG  | ASP | A | 549 | 25.703 | 68.058 | 86.214 | 1.00 | 22.44 |
|    | ATOM | 4394 | OD1 | ASP | A | 549 | 25.396 | 69.227 | 86.150 | 1.00 | 25.44 |
|    | ATOM | 4395 | OD2 | ASP | A | 549 | 26.252 | 67.575 | 87.271 | 1.00 | 25.86 |
|    | ATOM | 4396 | N   | ALA | A | 550 | 23.511 | 64.624 | 84.122 | 1.00 | 13.24 |
| 60 | ATOM | 4397 | CA  | ALA | A | 550 | 23.269 | 63.709 | 83.004 | 1.00 | 14.70 |
|    | ATOM | 4398 | C   | ALA | A | 550 | 21.845 | 63.707 | 82.473 | 1.00 | 17.89 |
|    | ATOM | 4399 | O   | ALA | A | 550 | 21.598 | 63.132 | 81.389 | 1.00 | 15.28 |
|    | ATOM | 4400 | CB  | ALA | A | 550 | 23.713 | 62.280 | 83.335 | 1.00 | 14.77 |
|    | ATOM | 4401 | N   | ILE | A | 551 | 20.926 | 64.308 | 83.251 | 1.00 | 16.18 |
|    | ATOM | 4402 | CA  | ILE | A | 551 | 19.497 | 64.377 | 82.914 | 1.00 | 16.05 |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
|    | ATOM | 4403 | C   | ILE | A | 551 | 19.182 | 64.894 | 81.523 | 1.00 | 18.70 |
|    | ATOM | 4404 | O   | ILE | A | 551 | 18.441 | 64.290 | 80.736 | 1.00 | 19.01 |
|    | ATOM | 4405 | CB  | ILE | A | 551 | 18.701 | 65.139 | 83.971 | 1.00 | 19.52 |
| 5  | ATOM | 4406 | CG1 | ILE | A | 551 | 18.692 | 64.281 | 85.232 | 1.00 | 20.39 |
|    | ATOM | 4407 | CG2 | ILE | A | 551 | 17.251 | 65.361 | 83.512 | 1.00 | 12.65 |
|    | ATOM | 4408 | CD1 | ILE | A | 551 | 18.167 | 64.995 | 86.485 | 1.00 | 15.78 |
|    | ATOM | 4409 | N   | PRO | A | 552 | 19.748 | 66.038 | 81.197 | 1.00 | 18.48 |
|    | ATOM | 4410 | CA  | PRO | A | 552 | 19.487 | 66.600 | 79.888 | 1.00 | 16.36 |
| 10 | ATOM | 4411 | C   | PRO | A | 552 | 20.084 | 65.736 | 78.795 | 1.00 | 19.64 |
|    | ATOM | 4412 | O   | PRO | A | 552 | 19.551 | 65.606 | 77.700 | 1.00 | 16.94 |
|    | ATOM | 4413 | CB  | PRO | A | 552 | 20.125 | 67.995 | 79.870 | 1.00 | 18.41 |
|    | ATOM | 4414 | CG  | PRO | A | 552 | 21.001 | 68.070 | 81.116 | 1.00 | 24.69 |
|    | ATOM | 4415 | CD  | PRO | A | 552 | 20.504 | 66.981 | 82.059 | 1.00 | 17.97 |
| 15 | ATOM | 4416 | N   | LEU | A | 553 | 21.226 | 65.144 | 79.075 | 1.00 | 17.67 |
|    | ATOM | 4417 | CA  | LEU | A | 553 | 21.852 | 64.302 | 78.072 | 1.00 | 15.47 |
|    | ATOM | 4418 | C   | LEU | A | 553 | 20.940 | 63.101 | 77.795 | 1.00 | 19.23 |
|    | ATOM | 4419 | O   | LEU | A | 553 | 20.704 | 62.655 | 76.681 | 1.00 | 16.64 |
|    | ATOM | 4420 | CB  | LEU | A | 553 | 23.275 | 63.819 | 78.501 | 1.00 | 13.81 |
| 20 | ATOM | 4421 | CG  | LEU | A | 553 | 24.239 | 64.905 | 79.002 | 1.00 | 19.25 |
|    | ATOM | 4422 | CD1 | LEU | A | 553 | 25.606 | 64.289 | 79.247 | 1.00 | 17.04 |
|    | ATOM | 4423 | CD2 | LEU | A | 553 | 24.412 | 65.997 | 77.955 | 1.00 | 18.39 |
|    | ATOM | 4424 | N   | ALA | A | 554 | 20.440 | 62.529 | 78.867 | 1.00 | 17.65 |
|    | ATOM | 4425 | CA  | ALA | A | 554 | 19.614 | 61.341 | 78.730 | 1.00 | 15.25 |
| 25 | ATOM | 4426 | C   | ALA | A | 554 | 18.330 | 61.673 | 78.029 | 1.00 | 19.37 |
|    | ATOM | 4427 | O   | ALA | A | 554 | 17.896 | 60.913 | 77.157 | 1.00 | 14.92 |
|    | ATOM | 4428 | CB  | ALA | A | 554 | 19.415 | 60.697 | 80.094 | 1.00 | 12.41 |
|    | ATOM | 4429 | N   | LEU | A | 555 | 17.746 | 62.821 | 78.410 | 1.00 | 14.59 |
|    | ATOM | 4430 | CA  | LEU | A | 555 | 16.514 | 63.224 | 77.750 | 1.00 | 17.50 |
| 30 | ATOM | 4431 | C   | LEU | A | 555 | 16.686 | 63.445 | 76.249 | 1.00 | 16.25 |
|    | ATOM | 4432 | O   | LEU | A | 555 | 15.822 | 63.168 | 75.435 | 1.00 | 15.71 |
|    | ATOM | 4433 | CB  | LEU | A | 555 | 15.921 | 64.531 | 78.318 | 1.00 | 18.40 |
|    | ATOM | 4434 | CG  | LEU | A | 555 | 15.298 | 64.374 | 79.695 | 1.00 | 23.82 |
|    | ATOM | 4435 | CD1 | LEU | A | 555 | 15.153 | 65.771 | 80.333 | 1.00 | 23.08 |
| 35 | ATOM | 4436 | CD2 | LEU | A | 555 | 13.934 | 63.692 | 79.583 | 1.00 | 18.63 |
|    | ATOM | 4437 | N   | LYS | A | 556 | 17.827 | 64.008 | 75.899 | 1.00 | 17.73 |
|    | ATOM | 4438 | CA  | LYS | A | 556 | 18.139 | 64.330 | 74.536 | 1.00 | 15.70 |
|    | ATOM | 4439 | C   | LYS | A | 556 | 18.285 | 63.076 | 73.702 | 1.00 | 19.09 |
|    | ATOM | 4440 | O   | LYS | A | 556 | 17.690 | 62.959 | 72.626 | 1.00 | 19.08 |
| 40 | ATOM | 4441 | CB  | LYS | A | 556 | 19.380 | 65.206 | 74.530 | 1.00 | 15.52 |
|    | ATOM | 4442 | CG  | LYS | A | 556 | 19.729 | 65.769 | 73.163 | 1.00 | 41.74 |
|    | ATOM | 4443 | CD  | LYS | A | 556 | 21.020 | 66.590 | 73.160 | 1.00 | 77.82 |
|    | ATOM | 4444 | CE  | LYS | A | 556 | 21.851 | 66.449 | 71.883 | 1.00 | 79.74 |
|    | ATOM | 4445 | NZ  | LYS | A | 556 | 22.446 | 67.709 | 71.404 | 1.00 | 60.52 |
| 45 | ATOM | 4446 | N   | MET | A | 557 | 19.089 | 62.128 | 74.207 | 1.00 | 15.27 |
|    | ATOM | 4447 | CA  | MET | A | 557 | 19.294 | 60.904 | 73.446 | 1.00 | 13.47 |
|    | ATOM | 4448 | C   | MET | A | 557 | 17.997 | 60.140 | 73.264 | 1.00 | 16.45 |
|    | ATOM | 4449 | O   | MET | A | 557 | 17.723 | 59.507 | 72.253 | 1.00 | 15.63 |
|    | ATOM | 4450 | CB  | MET | A | 557 | 20.312 | 59.998 | 74.165 | 1.00 | 14.26 |
| 50 | ATOM | 4451 | CG  | MET | A | 557 | 20.499 | 58.682 | 73.405 | 1.00 | 13.00 |
|    | ATOM | 4452 | SD  | MET | A | 557 | 21.984 | 57.796 | 73.915 | 1.00 | 16.44 |
|    | ATOM | 4453 | CE  | MET | A | 557 | 22.027 | 56.574 | 72.596 | 1.00 | 12.39 |
|    | ATOM | 4454 | N   | ALA | A | 558 | 17.200 | 60.181 | 74.327 | 1.00 | 18.08 |
|    | ATOM | 4455 | CA  | ALA | A | 558 | 15.955 | 59.438 | 74.323 | 1.00 | 17.49 |
| 55 | ATOM | 4456 | C   | ALA | A | 558 | 14.968 | 59.922 | 73.292 | 1.00 | 23.08 |
|    | ATOM | 4457 | O   | ALA | A | 558 | 14.221 | 59.153 | 72.723 | 1.00 | 21.14 |
|    | ATOM | 4458 | CB  | ALA | A | 558 | 15.316 | 59.439 | 75.705 | 1.00 | 16.55 |
|    | ATOM | 4459 | N   | THR | A | 559 | 14.951 | 61.220 | 73.082 | 1.00 | 18.89 |
|    | ATOM | 4460 | CA  | THR | A | 559 | 13.980 | 61.798 | 72.186 | 1.00 | 19.50 |
| 60 | ATOM | 4461 | C   | THR | A | 559 | 14.542 | 62.125 | 70.830 | 1.00 | 22.12 |
|    | ATOM | 4462 | O   | THR | A | 559 | 13.804 | 62.219 | 69.862 | 1.00 | 23.28 |
|    | ATOM | 4463 | CB  | THR | A | 559 | 13.418 | 63.078 | 72.824 | 1.00 | 25.23 |
|    | ATOM | 4464 | OG1 | THR | A | 559 | 14.493 | 63.999 | 73.001 | 1.00 | 22.20 |
|    | ATOM | 4465 | CG2 | THR | A | 559 | 12.734 | 62.723 | 74.147 | 1.00 | 18.19 |
|    | ATOM | 4466 | N   | GLU | A | 560 | 15.841 | 62.316 | 70.756 | 1.00 | 16.68 |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
|    | ATOM | 4467 | CA  | GLU | A | 560 | 16.399 | 62.646 | 69.479 | 1.00 | 18.60 |
|    | ATOM | 4468 | C   | GLU | A | 560 | 16.492 | 61.448 | 68.545 | 1.00 | 26.45 |
|    | ATOM | 4469 | O   | GLU | A | 560 | 16.714 | 61.608 | 67.344 | 1.00 | 21.93 |
| 5  | ATOM | 4470 | CB  | GLU | A | 560 | 17.748 | 63.317 | 69.640 | 1.00 | 21.55 |
|    | ATOM | 4471 | CG  | GLU | A | 560 | 17.623 | 64.757 | 70.136 | 1.00 | 38.31 |
|    | ATOM | 4472 | CD  | GLU | A | 560 | 18.990 | 65.352 | 70.221 | 1.00 | 55.37 |
|    | ATOM | 4473 | OE1 | GLU | A | 560 | 20.007 | 64.691 | 70.053 | 1.00 | 40.21 |
|    | ATOM | 4474 | OE2 | GLU | A | 560 | 18.946 | 66.627 | 70.504 | 1.00 | 55.04 |
| 10 | ATOM | 4475 | N   | GLN | A | 561 | 16.344 | 60.251 | 69.101 | 1.00 | 20.47 |
|    | ATOM | 4476 | CA  | GLN | A | 561 | 16.340 | 59.043 | 68.291 | 1.00 | 19.24 |
|    | ATOM | 4477 | C   | GLN | A | 561 | 15.283 | 58.189 | 68.921 | 1.00 | 18.06 |
|    | ATOM | 4478 | O   | GLN | A | 561 | 14.874 | 58.520 | 70.022 | 1.00 | 16.87 |
|    | ATOM | 4479 | CB  | GLN | A | 561 | 17.684 | 58.307 | 68.136 | 1.00 | 20.45 |
|    | ATOM | 4480 | CG  | GLN | A | 561 | 18.341 | 58.001 | 69.495 | 1.00 | 21.17 |
| 15 | ATOM | 4481 | CD  | GLN | A | 561 | 17.692 | 56.815 | 70.165 | 1.00 | 21.31 |
|    | ATOM | 4482 | OE1 | GLN | A | 561 | 17.302 | 56.877 | 71.344 | 1.00 | 23.07 |
|    | ATOM | 4483 | NE2 | GLN | A | 561 | 17.543 | 55.758 | 69.379 | 1.00 | 11.21 |
|    | ATOM | 4484 | N   | GLY | A | 562 | 14.821 | 57.148 | 68.239 | 1.00 | 16.15 |
|    | ATOM | 4485 | CA  | GLY | A | 562 | 13.758 | 56.367 | 68.827 | 1.00 | 14.79 |
| 20 | ATOM | 4486 | C   | GLY | A | 562 | 13.919 | 54.872 | 68.750 | 1.00 | 17.42 |
|    | ATOM | 4487 | O   | GLY | A | 562 | 12.941 | 54.134 | 68.842 | 1.00 | 22.06 |
|    | ATOM | 4488 | N   | ARG | A | 563 | 15.152 | 54.424 | 68.598 | 1.00 | 18.35 |
|    | ATOM | 4489 | CA  | ARG | A | 563 | 15.453 | 52.990 | 68.617 | 1.00 | 18.80 |
|    | ATOM | 4490 | C   | ARG | A | 563 | 15.023 | 52.501 | 70.018 | 1.00 | 16.67 |
| 25 | ATOM | 4491 | O   | ARG | A | 563 | 15.518 | 52.925 | 71.085 | 1.00 | 14.27 |
|    | ATOM | 4492 | CB  | ARG | A | 563 | 16.949 | 52.812 | 68.321 | 1.00 | 16.78 |
|    | ATOM | 4493 | CG  | ARG | A | 563 | 17.394 | 51.363 | 68.218 | 1.00 | 14.43 |
|    | ATOM | 4494 | CD  | ARG | A | 563 | 18.911 | 51.276 | 68.095 | 1.00 | 15.41 |
|    | ATOM | 4495 | NE  | ARG | A | 563 | 19.423 | 49.897 | 68.119 | 1.00 | 19.33 |
| 30 | ATOM | 4496 | CZ  | ARG | A | 563 | 20.683 | 49.669 | 67.774 | 1.00 | 19.66 |
|    | ATOM | 4497 | NH1 | ARG | A | 563 | 21.482 | 50.681 | 67.417 | 1.00 | 10.67 |
|    | ATOM | 4498 | NH2 | ARG | A | 563 | 21.148 | 48.428 | 67.779 | 1.00 | 13.38 |
|    | ATOM | 4499 | N   | MET | A | 564 | 14.003 | 51.648 | 70.069 | 1.00 | 13.84 |
|    | ATOM | 4500 | CA  | MET | A | 564 | 13.447 | 51.247 | 71.369 | 1.00 | 13.05 |
| 35 | ATOM | 4501 | C   | MET | A | 564 | 14.443 | 50.787 | 72.419 | 1.00 | 18.69 |
|    | ATOM | 4502 | O   | MET | A | 564 | 14.257 | 50.973 | 73.628 | 1.00 | 12.40 |
|    | ATOM | 4503 | CB  | MET | A | 564 | 12.315 | 50.212 | 71.198 | 1.00 | 13.81 |
|    | ATOM | 4504 | CG  | MET | A | 564 | 11.159 | 50.825 | 70.424 | 1.00 | 16.20 |
|    | ATOM | 4505 | SD  | MET | A | 564 | 9.692  | 49.805 | 70.530 | 1.00 | 21.23 |
| 40 | ATOM | 4506 | CE  | MET | A | 564 | 10.114 | 48.581 | 69.265 | 1.00 | 17.64 |
|    | ATOM | 4507 | N   | LYS | A | 565 | 15.464 | 50.097 | 71.892 | 1.00 | 16.37 |
|    | ATOM | 4508 | CA  | LYS | A | 565 | 16.521 | 49.537 | 72.701 | 1.00 | 13.75 |
|    | ATOM | 4509 | C   | LYS | A | 565 | 17.129 | 50.623 | 73.582 | 1.00 | 16.90 |
|    | ATOM | 4510 | O   | LYS | A | 565 | 17.493 | 50.376 | 74.735 | 1.00 | 14.97 |
| 45 | ATOM | 4511 | CB  | LYS | A | 565 | 17.549 | 48.885 | 71.767 | 1.00 | 11.37 |
|    | ATOM | 4512 | CG  | LYS | A | 565 | 18.793 | 48.371 | 72.459 | 1.00 | 12.72 |
|    | ATOM | 4513 | CD  | LYS | A | 565 | 19.962 | 48.100 | 71.525 | 1.00 | 17.72 |
|    | ATOM | 4514 | CE  | LYS | A | 565 | 21.060 | 47.336 | 72.239 | 1.00 | 19.39 |
|    | ATOM | 4515 | NZ  | LYS | A | 565 | 22.030 | 46.721 | 71.308 | 1.00 | 15.47 |
| 50 | ATOM | 4516 | N   | PHE | A | 566 | 17.211 | 51.847 | 73.057 | 1.00 | 12.01 |
|    | ATOM | 4517 | CA  | PHE | A | 566 | 17.801 | 52.912 | 73.846 | 1.00 | 12.25 |
|    | ATOM | 4518 | C   | PHE | A | 566 | 16.739 | 53.770 | 74.509 | 1.00 | 15.74 |
|    | ATOM | 4519 | O   | PHE | A | 566 | 16.843 | 54.177 | 75.661 | 1.00 | 12.91 |
|    | ATOM | 4520 | CB  | PHE | A | 566 | 18.641 | 53.814 | 72.932 | 1.00 | 12.87 |
| 55 | ATOM | 4521 | CG  | PHE | A | 566 | 19.744 | 53.117 | 72.165 | 1.00 | 14.44 |
|    | ATOM | 4522 | CD1 | PHE | A | 566 | 20.465 | 52.053 | 72.714 | 1.00 | 13.84 |
|    | ATOM | 4523 | CD2 | PHE | A | 566 | 20.111 | 53.577 | 70.894 | 1.00 | 15.31 |
|    | ATOM | 4524 | CE1 | PHE | A | 566 | 21.510 | 51.434 | 72.014 | 1.00 | 13.86 |
|    | ATOM | 4525 | CE2 | PHE | A | 566 | 21.145 | 52.977 | 70.172 | 1.00 | 14.39 |
| 60 | ATOM | 4526 | CZ  | PHE | A | 566 | 21.849 | 51.910 | 70.744 | 1.00 | 15.76 |
|    | ATOM | 4527 | N   | THR | A | 567 | 15.721 | 54.095 | 73.724 | 1.00 | 16.10 |
|    | ATOM | 4528 | CA  | THR | A | 567 | 14.642 | 54.966 | 74.184 | 1.00 | 14.70 |
|    | ATOM | 4529 | C   | THR | A | 567 | 13.876 | 54.518 | 75.423 | 1.00 | 14.32 |
|    | ATOM | 4530 | O   | THR | A | 567 | 13.615 | 55.315 | 76.346 | 1.00 | 14.88 |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
|    | ATOM | 4531 | CB  | THR | A | 567 | 13.707 | 55.409 | 73.030 | 1.00 | 14.81 |
|    | ATOM | 4532 | OG1 | THR | A | 567 | 14.465 | 56.204 | 72.148 | 1.00 | 15.28 |
|    | ATOM | 4533 | CG2 | THR | A | 567 | 12.520 | 56.196 | 73.596 | 1.00 | 14.89 |
| 5  | ATOM | 4534 | N   | ARG | A | 568 | 13.478 | 53.245 | 75.412 | 1.00 | 12.20 |
|    | ATOM | 4535 | CA  | ARG | A | 568 | 12.697 | 52.764 | 76.533 | 1.00 | 13.57 |
|    | ATOM | 4536 | C   | ARG | A | 568 | 13.393 | 52.797 | 77.876 | 1.00 | 14.85 |
|    | ATOM | 4537 | O   | ARG | A | 568 | 12.896 | 53.312 | 78.861 | 1.00 | 14.39 |
|    | ATOM | 4538 | CB  | ARG | A | 568 | 12.133 | 51.400 | 76.218 | 1.00 | 13.49 |
| 10 | ATOM | 4539 | CG  | ARG | A | 568 | 11.021 | 51.467 | 75.155 | 1.00 | 14.02 |
|    | ATOM | 4540 | CD  | ARG | A | 568 | 10.387 | 50.098 | 74.884 | 1.00 | 9.84  |
|    | ATOM | 4541 | NE  | ARG | A | 568 | 9.662  | 49.607 | 76.063 | 1.00 | 13.61 |
|    | ATOM | 4542 | CZ  | ARG | A | 568 | 9.236  | 48.368 | 76.197 | 1.00 | 17.32 |
|    | ATOM | 4543 | NH1 | ARG | A | 568 | 9.471  | 47.427 | 75.275 | 1.00 | 13.23 |
| 15 | ATOM | 4544 | NH2 | ARG | A | 568 | 8.566  | 48.053 | 77.293 | 1.00 | 13.32 |
|    | ATOM | 4545 | N   | PRO | A | 569 | 14.577 | 52.237 | 77.948 | 1.00 | 12.95 |
|    | ATOM | 4546 | CA  | PRO | A | 569 | 15.294 | 52.206 | 79.229 | 1.00 | 10.82 |
|    | ATOM | 4547 | C   | PRO | A | 569 | 15.810 | 53.574 | 79.653 | 1.00 | 15.13 |
|    | ATOM | 4548 | O   | PRO | A | 569 | 15.977 | 53.859 | 80.849 | 1.00 | 14.45 |
| 20 | ATOM | 4549 | CB  | PRO | A | 569 | 16.479 | 51.262 | 79.000 | 1.00 | 14.29 |
|    | ATOM | 4550 | CG  | PRO | A | 569 | 16.245 | 50.553 | 77.659 | 1.00 | 17.55 |
|    | ATOM | 4551 | CD  | PRO | A | 569 | 15.224 | 51.385 | 76.897 | 1.00 | 16.15 |
|    | ATOM | 4552 | N   | LEU | A | 570 | 16.069 | 54.462 | 78.685 | 1.00 | 15.08 |
|    | ATOM | 4553 | CA  | LEU | A | 570 | 16.502 | 55.813 | 79.082 | 1.00 | 16.35 |
| 25 | ATOM | 4554 | C   | LEU | A | 570 | 15.321 | 56.509 | 79.784 | 1.00 | 19.34 |
|    | ATOM | 4555 | O   | LEU | A | 570 | 15.401 | 57.045 | 80.898 | 1.00 | 16.13 |
|    | ATOM | 4556 | CB  | LEU | A | 570 | 16.944 | 56.615 | 77.840 | 1.00 | 16.51 |
|    | ATOM | 4557 | CG  | LEU | A | 570 | 18.372 | 56.269 | 77.386 | 1.00 | 18.67 |
|    | ATOM | 4558 | CD1 | LEU | A | 570 | 18.737 | 57.028 | 76.110 | 1.00 | 16.85 |
| 30 | ATOM | 4559 | CD2 | LEU | A | 570 | 19.392 | 56.601 | 78.486 | 1.00 | 14.01 |
|    | ATOM | 4560 | N   | PHE | A | 571 | 14.161 | 56.435 | 79.129 | 1.00 | 14.02 |
|    | ATOM | 4561 | CA  | PHE | A | 571 | 12.978 | 57.007 | 79.732 | 1.00 | 14.67 |
|    | ATOM | 4562 | C   | PHE | A | 571 | 12.684 | 56.323 | 81.054 | 1.00 | 18.94 |
|    | ATOM | 4563 | O   | PHE | A | 571 | 12.257 | 56.933 | 82.030 | 1.00 | 18.09 |
| 35 | ATOM | 4564 | CB  | PHE | A | 571 | 11.721 | 56.805 | 78.872 | 1.00 | 14.94 |
|    | ATOM | 4565 | CG  | PHE | A | 571 | 11.462 | 57.993 | 78.014 | 1.00 | 17.38 |
|    | ATOM | 4566 | CD1 | PHE | A | 571 | 11.035 | 59.194 | 78.591 | 1.00 | 18.00 |
|    | ATOM | 4567 | CD2 | PHE | A | 571 | 11.634 | 57.902 | 76.633 | 1.00 | 19.72 |
|    | ATOM | 4568 | CE1 | PHE | A | 571 | 10.768 | 60.317 | 77.805 | 1.00 | 17.86 |
| 40 | ATOM | 4569 | CE2 | PHE | A | 571 | 11.358 | 59.016 | 75.836 | 1.00 | 23.80 |
|    | ATOM | 4570 | CZ  | PHE | A | 571 | 10.933 | 60.213 | 76.422 | 1.00 | 22.47 |
|    | ATOM | 4571 | N   | LYS | A | 572 | 12.839 | 55.023 | 81.080 | 1.00 | 14.21 |
|    | ATOM | 4572 | CA  | LYS | A | 572 | 12.530 | 54.361 | 82.325 | 1.00 | 14.07 |
|    | ATOM | 4573 | C   | LYS | A | 572 | 13.476 | 54.788 | 83.444 | 1.00 | 16.22 |
| 45 | ATOM | 4574 | O   | LYS | A | 572 | 13.123 | 54.998 | 84.620 | 1.00 | 16.74 |
|    | ATOM | 4575 | CB  | LYS | A | 572 | 12.533 | 52.850 | 82.147 | 1.00 | 15.58 |
|    | ATOM | 4576 | CG  | LYS | A | 572 | 11.179 | 52.157 | 82.243 | 1.00 | 32.41 |
|    | ATOM | 4577 | CD  | LYS | A | 572 | 11.197 | 50.722 | 81.697 | 1.00 | 46.79 |
|    | ATOM | 4578 | CE  | LYS | A | 572 | 11.249 | 50.620 | 80.160 | 1.00 | 56.38 |
| 50 | ATOM | 4579 | NZ  | LYS | A | 572 | 11.823 | 49.373 | 79.593 | 1.00 | 42.31 |
|    | ATOM | 4580 | N   | ASP | A | 573 | 14.735 | 54.914 | 83.089 | 1.00 | 14.00 |
|    | ATOM | 4581 | CA  | ASP | A | 573 | 15.671 | 55.286 | 84.148 | 1.00 | 15.33 |
|    | ATOM | 4582 | C   | ASP | A | 573 | 15.394 | 56.675 | 84.662 | 1.00 | 15.63 |
|    | ATOM | 4583 | O   | ASP | A | 573 | 15.531 | 56.959 | 85.850 | 1.00 | 15.64 |
| 55 | ATOM | 4584 | CB  | ASP | A | 573 | 17.137 | 55.288 | 83.627 | 1.00 | 14.94 |
|    | ATOM | 4585 | CG  | ASP | A | 573 | 17.688 | 53.889 | 83.452 | 1.00 | 22.26 |
|    | ATOM | 4586 | OD1 | ASP | A | 573 | 17.054 | 52.891 | 83.773 | 1.00 | 18.66 |
|    | ATOM | 4587 | OD2 | ASP | A | 573 | 18.923 | 53.848 | 82.983 | 1.00 | 18.27 |
|    | ATOM | 4588 | N   | LEU | A | 574 | 15.090 | 57.554 | 83.708 | 1.00 | 12.68 |
| 60 | ATOM | 4589 | CA  | LEU | A | 574 | 14.851 | 58.926 | 84.092 | 1.00 | 11.33 |
|    | ATOM | 4590 | C   | LEU | A | 574 | 13.611 | 59.053 | 84.970 | 1.00 | 22.78 |
|    | ATOM | 4591 | O   | LEU | A | 574 | 13.513 | 59.923 | 85.837 | 1.00 | 18.71 |
|    | ATOM | 4592 | CB  | LEU | A | 574 | 14.682 | 59.802 | 82.863 | 1.00 | 10.39 |
|    | ATOM | 4593 | CG  | LEU | A | 574 | 15.953 | 60.021 | 82.061 | 1.00 | 16.41 |
|    | ATOM | 4594 | CD1 | LEU | A | 574 | 15.501 | 60.352 | 80.630 | 1.00 | 16.48 |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
|    | ATOM | 4595 | CD2 | LEU | A | 574 | 16.785 | 61.200 | 82.608 | 1.00 | 12.08 |
|    | ATOM | 4596 | N   | ALA | A | 575 | 12.638 | 58.173 | 84.726 | 1.00 | 17.79 |
|    | ATOM | 4597 | CA  | ALA | A | 575 | 11.437 | 58.235 | 85.500 | 1.00 | 15.87 |
| 5  | ATOM | 4598 | C   | ALA | A | 575 | 11.720 | 57.682 | 86.856 | 1.00 | 17.98 |
|    | ATOM | 4599 | O   | ALA | A | 575 | 11.050 | 58.033 | 87.801 | 1.00 | 17.45 |
|    | ATOM | 4600 | CB  | ALA | A | 575 | 10.325 | 57.449 | 84.820 | 1.00 | 17.20 |
|    | ATOM | 4601 | N   | ALA | A | 576 | 12.703 | 56.801 | 86.972 | 1.00 | 14.91 |
|    | ATOM | 4602 | CA  | ALA | A | 576 | 13.024 | 56.222 | 88.272 | 1.00 | 12.59 |
| 10 | ATOM | 4603 | C   | ALA | A | 576 | 13.930 | 57.135 | 89.097 | 1.00 | 19.97 |
|    | ATOM | 4604 | O   | ALA | A | 576 | 14.140 | 56.920 | 90.281 | 1.00 | 22.87 |
|    | ATOM | 4605 | CB  | ALA | A | 576 | 13.732 | 54.881 | 88.146 | 1.00 | 16.01 |
|    | ATOM | 4606 | N   | PHE | A | 577 | 14.474 | 58.152 | 88.469 | 1.00 | 15.13 |
|    | ATOM | 4607 | CA  | PHE | A | 577 | 15.337 | 59.105 | 89.161 | 1.00 | 15.19 |
| 15 | ATOM | 4608 | C   | PHE | A | 577 | 14.412 | 60.219 | 89.660 | 1.00 | 19.07 |
|    | ATOM | 4609 | O   | PHE | A | 577 | 13.790 | 60.932 | 88.868 | 1.00 | 16.74 |
|    | ATOM | 4610 | CB  | PHE | A | 577 | 16.447 | 59.652 | 88.210 | 1.00 | 14.02 |
|    | ATOM | 4611 | CG  | PHE | A | 577 | 17.494 | 60.595 | 88.820 | 1.00 | 15.39 |
|    | ATOM | 4612 | CD1 | PHE | A | 577 | 17.678 | 60.707 | 90.202 | 1.00 | 17.32 |
| 20 | ATOM | 4613 | CD2 | PHE | A | 577 | 18.295 | 61.380 | 87.983 | 1.00 | 15.42 |
|    | ATOM | 4614 | CE1 | PHE | A | 577 | 18.646 | 61.570 | 90.727 | 1.00 | 18.05 |
|    | ATOM | 4615 | CE2 | PHE | A | 577 | 19.272 | 62.236 | 88.483 | 1.00 | 18.23 |
|    | ATOM | 4616 | CZ  | PHE | A | 577 | 19.442 | 62.330 | 89.866 | 1.00 | 18.02 |
|    | ATOM | 4617 | N   | ASP | A | 578 | 14.285 | 60.335 | 90.983 | 1.00 | 19.21 |
| 25 | ATOM | 4618 | CA  | ASP | A | 578 | 13.394 | 61.327 | 91.584 | 1.00 | 19.27 |
|    | ATOM | 4619 | C   | ASP | A | 578 | 13.568 | 62.692 | 90.981 | 1.00 | 18.95 |
|    | ATOM | 4620 | O   | ASP | A | 578 | 12.577 | 63.347 | 90.660 | 1.00 | 18.48 |
|    | ATOM | 4621 | CB  | ASP | A | 578 | 13.457 | 61.342 | 93.130 | 1.00 | 28.60 |
|    | ATOM | 4622 | CG  | ASP | A | 578 | 14.714 | 61.992 | 93.690 | 1.00 | 55.79 |
| 30 | ATOM | 4623 | OD1 | ASP | A | 578 | 15.779 | 62.135 | 93.064 | 1.00 | 45.74 |
|    | ATOM | 4624 | OD2 | ASP | A | 578 | 14.512 | 62.401 | 94.929 | 1.00 | 67.85 |
|    | ATOM | 4625 | N   | LYS | A | 579 | 14.839 | 63.083 | 90.791 | 1.00 | 17.12 |
|    | ATOM | 4626 | CA  | LYS | A | 579 | 15.185 | 64.352 | 90.194 | 1.00 | 13.88 |
|    | ATOM | 4627 | C   | LYS | A | 579 | 14.693 | 64.569 | 88.758 | 1.00 | 21.03 |
| 35 | ATOM | 4628 | O   | LYS | A | 579 | 14.338 | 65.689 | 88.386 | 1.00 | 20.91 |
|    | ATOM | 4629 | CB  | LYS | A | 579 | 16.669 | 64.621 | 90.293 | 1.00 | 13.46 |
|    | ATOM | 4630 | CG  | LYS | A | 579 | 17.159 | 64.570 | 91.724 | 1.00 | 33.01 |
|    | ATOM | 4631 | CD  | LYS | A | 579 | 16.890 | 65.878 | 92.442 | 1.00 | 55.78 |
|    | ATOM | 4632 | CE  | LYS | A | 579 | 16.292 | 65.662 | 93.816 | 1.00 | 58.11 |
| 40 | ATOM | 4633 | NZ  | LYS | A | 579 | 17.121 | 66.260 | 94.867 | 1.00 | 54.50 |
|    | ATOM | 4634 | N   | SER | A | 580 | 14.646 | 63.553 | 87.897 | 1.00 | 14.45 |
|    | ATOM | 4635 | CA  | SER | A | 580 | 14.187 | 63.844 | 86.540 | 1.00 | 13.57 |
|    | ATOM | 4636 | C   | SER | A | 580 | 12.798 | 63.298 | 86.228 | 1.00 | 20.81 |
|    | ATOM | 4637 | O   | SER | A | 580 | 12.313 | 63.384 | 85.103 | 1.00 | 19.66 |
| 45 | ATOM | 4638 | CB  | SER | A | 580 | 15.113 | 63.091 | 85.601 | 1.00 | 12.97 |
|    | ATOM | 4639 | OG  | SER | A | 580 | 15.350 | 61.809 | 86.186 | 1.00 | 17.95 |
|    | ATOM | 4640 | N   | HIS | A | 581 | 12.184 | 62.664 | 87.196 | 1.00 | 16.52 |
|    | ATOM | 4641 | CA  | HIS | A | 581 | 10.897 | 62.042 | 86.971 | 1.00 | 16.52 |
|    | ATOM | 4642 | C   | HIS | A | 581 | 9.816  | 62.866 | 86.281 | 1.00 | 21.39 |
| 50 | ATOM | 4643 | O   | HIS | A | 581 | 9.250  | 62.522 | 85.234 | 1.00 | 18.75 |
|    | ATOM | 4644 | CB  | HIS | A | 581 | 10.389 | 61.487 | 88.289 | 1.00 | 15.62 |
|    | ATOM | 4645 | CG  | HIS | A | 581 | 9.034  | 60.927 | 88.100 | 1.00 | 22.66 |
|    | ATOM | 4646 | ND1 | HIS | A | 581 | 7.914  | 61.748 | 88.110 | 1.00 | 27.83 |
|    | ATOM | 4647 | CD2 | HIS | A | 581 | 8.623  | 59.644 | 87.899 | 1.00 | 27.04 |
| 55 | ATOM | 4648 | CE1 | HIS | A | 581 | 6.843  | 60.975 | 87.926 | 1.00 | 27.26 |
|    | ATOM | 4649 | NE2 | HIS | A | 581 | 7.242  | 59.715 | 87.789 | 1.00 | 28.84 |
|    | ATOM | 4650 | N   | ASP | A | 582 | 9.515  | 63.986 | 86.884 | 1.00 | 17.59 |
|    | ATOM | 4651 | CA  | ASP | A | 582 | 8.491  | 64.831 | 86.322 | 1.00 | 20.99 |
|    | ATOM | 4652 | C   | ASP | A | 582 | 8.831  | 65.284 | 84.927 | 1.00 | 24.43 |
| 60 | ATOM | 4653 | O   | ASP | A | 582 | 8.013  | 65.343 | 84.030 | 1.00 | 21.69 |
|    | ATOM | 4654 | CB  | ASP | A | 582 | 8.331  | 66.085 | 87.197 | 1.00 | 25.08 |
|    | ATOM | 4655 | CG  | ASP | A | 582 | 7.626  | 65.730 | 88.466 | 1.00 | 30.98 |
|    | ATOM | 4656 | OD1 | ASP | A | 582 | 7.129  | 64.638 | 88.645 | 1.00 | 36.19 |
|    | ATOM | 4657 | OD2 | ASP | A | 582 | 7.659  | 66.680 | 89.359 | 1.00 | 38.67 |
|    | ATOM | 4658 | N   | GLN | A | 583 | 10.075 | 65.649 | 84.762 | 1.00 | 20.38 |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5  | ATOM | 4659 | CA  | GLN | A | 583 | 10.451 | 66.076 | 83.465 | 1.00 | 19.54 |
|    | ATOM | 4660 | C   | GLN | A | 583 | 10.423 | 64.938 | 82.431 | 1.00 | 23.45 |
|    | ATOM | 4661 | O   | GLN | A | 583 | 10.182 | 65.148 | 81.229 | 1.00 | 23.51 |
|    | ATOM | 4662 | CB  | GLN | A | 583 | 11.857 | 66.642 | 83.573 | 1.00 | 19.50 |
|    | ATOM | 4663 | CG  | GLN | A | 583 | 12.188 | 67.300 | 82.240 | 1.00 | 21.61 |
| 10 | ATOM | 4664 | CD  | GLN | A | 583 | 13.503 | 68.019 | 82.370 | 1.00 | 44.67 |
|    | ATOM | 4665 | OE1 | GLN | A | 583 | 14.236 | 67.818 | 83.357 | 1.00 | 39.11 |
|    | ATOM | 4666 | NE2 | GLN | A | 583 | 13.778 | 68.840 | 81.373 | 1.00 | 40.61 |
|    | ATOM | 4667 | N   | ALA | A | 584 | 10.706 | 63.718 | 82.866 | 1.00 | 18.70 |
|    | ATOM | 4668 | CA  | ALA | A | 584 | 10.700 | 62.595 | 81.927 | 1.00 | 15.00 |
| 15 | ATOM | 4669 | C   | ALA | A | 584 | 9.307  | 62.411 | 81.375 | 1.00 | 19.16 |
|    | ATOM | 4670 | O   | ALA | A | 584 | 9.101  | 62.211 | 80.176 | 1.00 | 19.25 |
|    | ATOM | 4671 | CB  | ALA | A | 584 | 11.043 | 61.288 | 82.642 | 1.00 | 13.44 |
|    | ATOM | 4672 | N   | VAL | A | 585 | 8.356  | 62.452 | 82.316 | 1.00 | 15.46 |
|    | ATOM | 4673 | CA  | VAL | A | 585 | 6.941  | 62.258 | 81.999 | 1.00 | 18.57 |
| 20 | ATOM | 4674 | C   | VAL | A | 585 | 6.418  | 63.339 | 81.064 | 1.00 | 25.46 |
|    | ATOM | 4675 | O   | VAL | A | 585 | 5.743  | 63.106 | 80.055 | 1.00 | 23.63 |
|    | ATOM | 4676 | CB  | VAL | A | 585 | 6.090  | 62.120 | 83.274 | 1.00 | 23.07 |
|    | ATOM | 4677 | CG1 | VAL | A | 585 | 4.610  | 62.298 | 82.946 | 1.00 | 23.53 |
|    | ATOM | 4678 | CG2 | VAL | A | 585 | 6.340  | 60.775 | 83.966 | 1.00 | 21.15 |
| 25 | ATOM | 4679 | N   | ARG | A | 586 | 6.792  | 64.564 | 81.405 | 1.00 | 23.81 |
|    | ATOM | 4680 | CA  | ARG | A | 586 | 6.395  | 65.688 | 80.615 | 1.00 | 22.41 |
|    | ATOM | 4681 | C   | ARG | A | 586 | 6.974  | 65.628 | 79.223 | 1.00 | 22.13 |
|    | ATOM | 4682 | O   | ARG | A | 586 | 6.283  | 65.909 | 78.254 | 1.00 | 20.69 |
|    | ATOM | 4683 | CB  | ARG | A | 586 | 6.695  | 67.000 | 81.329 | 1.00 | 21.27 |
| 30 | ATOM | 4684 | CG  | ARG | A | 586 | 6.573  | 68.251 | 80.461 | 1.00 | 39.32 |
|    | ATOM | 4685 | CD  | ARG | A | 586 | 7.134  | 69.519 | 81.129 | 1.00 | 45.58 |
|    | ATOM | 4686 | NE  | ARG | A | 586 | 7.498  | 69.270 | 82.525 | 1.00 | 68.78 |
|    | ATOM | 4687 | CZ  | ARG | A | 586 | 8.712  | 69.427 | 83.074 | 1.00 | 82.97 |
|    | ATOM | 4688 | NH1 | ARG | A | 586 | 9.767  | 69.873 | 82.357 | 1.00 | 50.55 |
| 35 | ATOM | 4689 | NH2 | ARG | A | 586 | 8.842  | 69.129 | 84.383 | 1.00 | 31.22 |
|    | ATOM | 4690 | N   | THR | A | 587 | 8.231  | 65.247 | 79.095 | 1.00 | 19.40 |
|    | ATOM | 4691 | CA  | THR | A | 587 | 8.856  | 65.157 | 77.781 | 1.00 | 18.84 |
|    | ATOM | 4692 | C   | THR | A | 587 | 8.150  | 64.170 | 76.882 | 1.00 | 20.71 |
|    | ATOM | 4693 | O   | THR | A | 587 | 7.885  | 64.391 | 75.702 | 1.00 | 23.03 |
| 40 | ATOM | 4694 | CB  | THR | A | 587 | 10.313 | 64.746 | 77.975 | 1.00 | 23.70 |
|    | ATOM | 4695 | OG1 | THR | A | 587 | 10.887 | 65.693 | 78.846 | 1.00 | 21.83 |
|    | ATOM | 4696 | CG2 | THR | A | 587 | 11.048 | 64.672 | 76.654 | 1.00 | 21.38 |
|    | ATOM | 4697 | N   | TYR | A | 588 | 7.822  | 63.043 | 77.464 | 1.00 | 21.74 |
|    | ATOM | 4698 | CA  | TYR | A | 588 | 7.137  | 62.033 | 76.693 | 1.00 | 19.43 |
| 45 | ATOM | 4699 | C   | TYR | A | 588 | 5.808  | 62.573 | 76.151 | 1.00 | 24.31 |
|    | ATOM | 4700 | O   | TYR | A | 588 | 5.450  | 62.483 | 74.963 | 1.00 | 26.68 |
|    | ATOM | 4701 | CB  | TYR | A | 588 | 6.846  | 60.854 | 77.638 | 1.00 | 18.46 |
|    | ATOM | 4702 | CG  | TYR | A | 588 | 5.842  | 59.904 | 77.014 | 1.00 | 21.76 |
|    | ATOM | 4703 | CD1 | TYR | A | 588 | 6.169  | 59.136 | 75.891 | 1.00 | 22.44 |
| 50 | ATOM | 4704 | CD2 | TYR | A | 588 | 4.549  | 59.808 | 77.540 | 1.00 | 22.19 |
|    | ATOM | 4705 | CE1 | TYR | A | 588 | 5.217  | 58.274 | 75.335 | 1.00 | 26.93 |
|    | ATOM | 4706 | CE2 | TYR | A | 588 | 3.584  | 58.961 | 76.999 | 1.00 | 19.19 |
|    | ATOM | 4707 | CZ  | TYR | A | 588 | 3.936  | 58.191 | 75.890 | 1.00 | 25.45 |
|    | ATOM | 4708 | OH  | TYR | A | 588 | 3.008  | 57.335 | 75.359 | 1.00 | 24.42 |
| 55 | ATOM | 4709 | N   | GLN | A | 589 | 5.039  | 63.110 | 77.088 | 1.00 | 23.42 |
|    | ATOM | 4710 | CA  | GLN | A | 589 | 3.727  | 63.642 | 76.762 | 1.00 | 22.93 |
|    | ATOM | 4711 | C   | GLN | A | 589 | 3.806  | 64.594 | 75.596 | 1.00 | 20.18 |
|    | ATOM | 4712 | O   | GLN | A | 589 | 2.957  | 64.626 | 74.707 | 1.00 | 23.55 |
|    | ATOM | 4713 | CB  | GLN | A | 589 | 3.139  | 64.384 | 77.981 | 1.00 | 25.07 |
| 60 | ATOM | 4714 | CG  | GLN | A | 589 | 2.683  | 63.449 | 79.119 | 1.00 | 21.54 |
|    | ATOM | 4715 | CD  | GLN | A | 589 | 1.470  | 62.587 | 78.765 | 1.00 | 41.81 |
|    | ATOM | 4716 | OE1 | GLN | A | 589 | 1.197  | 62.264 | 77.606 | 1.00 | 37.70 |
|    | ATOM | 4717 | NE2 | GLN | A | 589 | 0.721  | 62.186 | 79.779 | 1.00 | 58.94 |
|    | ATOM | 4718 | N   | GLU | A | 590 | 4.844  | 65.400 | 75.649 | 1.00 | 17.93 |
|    | ATOM | 4719 | CA  | GLU | A | 590 | 5.097  | 66.416 | 74.644 | 1.00 | 19.01 |
|    | ATOM | 4720 | C   | GLU | A | 590 | 5.566  | 65.826 | 73.363 | 1.00 | 26.93 |
|    | ATOM | 4721 | O   | GLU | A | 590 | 5.393  | 66.453 | 72.312 | 1.00 | 23.86 |
|    | ATOM | 4722 | CB  | GLU | A | 590 | 6.176  | 67.452 | 75.021 | 1.00 | 20.73 |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
|    | ATOM | 4723 | CG  | GLU | A | 590 | 5.706  | 68.358 | 76.180 | 1.00 | 36.88 |
|    | ATOM | 4724 | CD  | GLU | A | 590 | 6.810  | 69.187 | 76.769 | 1.00 | 62.73 |
|    | ATOM | 4725 | OE1 | GLU | A | 590 | 7.988  | 69.112 | 76.403 | 1.00 | 55.19 |
| 5  | ATOM | 4726 | OE2 | GLU | A | 590 | 6.341  | 69.975 | 77.718 | 1.00 | 40.10 |
|    | ATOM | 4727 | N   | HIS | A | 591 | 6.203  | 64.666 | 73.476 | 1.00 | 23.79 |
|    | ATOM | 4728 | CA  | HIS | A | 591 | 6.700  | 64.086 | 72.250 | 1.00 | 23.24 |
|    | ATOM | 4729 | C   | HIS | A | 591 | 5.818  | 63.013 | 71.689 | 1.00 | 20.50 |
|    | ATOM | 4730 | O   | HIS | A | 591 | 5.965  | 62.619 | 70.541 | 1.00 | 24.92 |
| 10 | ATOM | 4731 | CB  | HIS | A | 591 | 8.076  | 63.446 | 72.481 | 1.00 | 22.84 |
|    | ATOM | 4732 | CG  | HIS | A | 591 | 9.175  | 64.446 | 72.384 | 1.00 | 25.11 |
|    | ATOM | 4733 | ND1 | HIS | A | 591 | 9.381  | 65.385 | 73.378 | 1.00 | 28.84 |
|    | ATOM | 4734 | CD2 | HIS | A | 591 | 10.092 | 64.667 | 71.403 | 1.00 | 26.79 |
|    | ATOM | 4735 | CE1 | HIS | A | 591 | 10.408 | 66.147 | 72.984 | 1.00 | 27.18 |
|    | ATOM | 4736 | NE2 | HIS | A | 591 | 10.853 | 65.745 | 71.796 | 1.00 | 26.51 |
| 15 | ATOM | 4737 | N   | LYS | A | 592 | 4.939  | 62.487 | 72.503 | 1.00 | 19.36 |
|    | ATOM | 4738 | CA  | LYS | A | 592 | 4.202  | 61.366 | 71.988 | 1.00 | 19.14 |
|    | ATOM | 4739 | C   | LYS | A | 592 | 3.553  | 61.382 | 70.613 | 1.00 | 28.03 |
|    | ATOM | 4740 | O   | LYS | A | 592 | 3.592  | 60.409 | 69.856 | 1.00 | 23.29 |
| 20 | ATOM | 4741 | CB  | LYS | A | 592 | 3.431  | 60.669 | 73.048 | 1.00 | 18.80 |
|    | ATOM | 4742 | CG  | LYS | A | 592 | 2.321  | 61.545 | 73.519 | 1.00 | 26.37 |
|    | ATOM | 4743 | CD  | LYS | A | 592 | 1.414  | 60.713 | 74.400 | 1.00 | 33.29 |
|    | ATOM | 4744 | CE  | LYS | A | 592 | 0.018  | 61.301 | 74.523 | 1.00 | 45.98 |
|    | ATOM | 4745 | NZ  | LYS | A | 592 | -0.530 | 61.163 | 75.874 | 1.00 | 25.02 |
| 25 | ATOM | 4746 | N   | ALA | A | 593 | 2.905  | 62.494 | 70.300 | 1.00 | 29.63 |
|    | ATOM | 4747 | CA  | ALA | A | 593 | 2.225  | 62.650 | 69.016 | 1.00 | 26.27 |
|    | ATOM | 4748 | C   | ALA | A | 593 | 3.157  | 62.524 | 67.808 | 1.00 | 26.27 |
|    | ATOM | 4749 | O   | ALA | A | 593 | 2.741  | 62.121 | 66.732 | 1.00 | 28.39 |
|    | ATOM | 4750 | CB  | ALA | A | 593 | 1.558  | 64.018 | 68.998 | 1.00 | 24.94 |
| 30 | ATOM | 4751 | N   | SER | A | 594 | 4.420  | 62.891 | 67.988 | 1.00 | 21.56 |
|    | ATOM | 4752 | CA  | SER | A | 594 | 5.404  | 62.867 | 66.930 | 1.00 | 22.18 |
|    | ATOM | 4753 | C   | SER | A | 594 | 6.238  | 61.590 | 66.949 | 1.00 | 22.38 |
|    | ATOM | 4754 | O   | SER | A | 594 | 7.160  | 61.444 | 66.137 | 1.00 | 20.87 |
|    | ATOM | 4755 | CB  | SER | A | 594 | 6.352  | 64.049 | 67.098 | 1.00 | 29.27 |
| 35 | ATOM | 4756 | OG  | SER | A | 594 | 7.286  | 63.814 | 68.156 | 1.00 | 45.26 |
|    | ATOM | 4757 | N   | MET | A | 595 | 5.922  | 60.678 | 67.858 | 1.00 | 17.72 |
|    | ATOM | 4758 | CA  | MET | A | 595 | 6.732  | 59.453 | 67.945 | 1.00 | 17.90 |
|    | ATOM | 4759 | C   | MET | A | 595 | 6.240  | 58.295 | 67.114 | 1.00 | 21.97 |
|    | ATOM | 4760 | O   | MET | A | 595 | 5.105  | 58.257 | 66.683 | 1.00 | 26.36 |
| 40 | ATOM | 4761 | CB  | MET | A | 595 | 6.717  | 58.931 | 69.396 | 1.00 | 17.35 |
|    | ATOM | 4762 | CG  | MET | A | 595 | 7.616  | 59.720 | 70.321 | 1.00 | 18.64 |
|    | ATOM | 4763 | SD  | MET | A | 595 | 7.451  | 59.068 | 71.999 | 1.00 | 25.54 |
|    | ATOM | 4764 | CE  | MET | A | 595 | 7.775  | 60.523 | 72.990 | 1.00 | 32.21 |
|    | ATOM | 4765 | N   | HIS | A | 596 | 7.066  | 57.284 | 66.954 | 1.00 | 15.02 |
| 45 | ATOM | 4766 | CA  | HIS | A | 596 | 6.593  | 56.105 | 66.258 | 1.00 | 16.62 |
|    | ATOM | 4767 | C   | HIS | A | 596 | 5.458  | 55.524 | 67.111 | 1.00 | 19.77 |
|    | ATOM | 4768 | O   | HIS | A | 596 | 5.474  | 55.605 | 68.324 | 1.00 | 19.53 |
|    | ATOM | 4769 | CB  | HIS | A | 596 | 7.756  | 55.103 | 66.052 | 1.00 | 17.44 |
|    | ATOM | 4770 | CG  | HIS | A | 596 | 7.280  | 53.844 | 65.414 | 1.00 | 20.36 |
| 50 | ATOM | 4771 | ND1 | HIS | A | 596 | 7.474  | 53.623 | 64.059 | 1.00 | 22.76 |
|    | ATOM | 4772 | CD2 | HIS | A | 596 | 6.582  | 52.790 | 65.937 | 1.00 | 19.37 |
|    | ATOM | 4773 | CE1 | HIS | A | 596 | 6.928  | 52.443 | 63.770 | 1.00 | 21.23 |
|    | ATOM | 4774 | NE2 | HIS | A | 596 | 6.375  | 51.935 | 64.879 | 1.00 | 22.61 |
|    | ATOM | 4775 | N   | PRO | A | 597 | 4.425  | 54.948 | 66.507 | 1.00 | 19.72 |
| 55 | ATOM | 4776 | CA  | PRO | A | 597 | 3.284  | 54.409 | 67.233 | 1.00 | 17.32 |
|    | ATOM | 4777 | C   | PRO | A | 597 | 3.515  | 53.268 | 68.221 | 1.00 | 22.24 |
|    | ATOM | 4778 | O   | PRO | A | 597 | 2.887  | 53.165 | 69.277 | 1.00 | 20.86 |
|    | ATOM | 4779 | CB  | PRO | A | 597 | 2.228  | 54.031 | 66.181 | 1.00 | 15.13 |
|    | ATOM | 4780 | CG  | PRO | A | 597 | 2.989  | 53.918 | 64.893 | 1.00 | 20.16 |
| 60 | ATOM | 4781 | CD  | PRO | A | 597 | 4.195  | 54.843 | 65.045 | 1.00 | 19.53 |
|    | ATOM | 4782 | N   | VAL | A | 598 | 4.381  | 52.340 | 67.895 | 1.00 | 17.95 |
|    | ATOM | 4783 | CA  | VAL | A | 598 | 4.575  | 51.277 | 68.868 | 1.00 | 17.06 |
|    | ATOM | 4784 | C   | VAL | A | 598 | 5.463  | 51.830 | 69.993 | 1.00 | 16.39 |
|    | ATOM | 4785 | O   | VAL | A | 598 | 5.188  | 51.629 | 71.176 | 1.00 | 18.72 |
|    | ATOM | 4786 | CB  | VAL | A | 598 | 5.175  | 50.039 | 68.180 | 1.00 | 20.87 |



|    |      |      |     |     |   |     |       |        |        |      |       |
|----|------|------|-----|-----|---|-----|-------|--------|--------|------|-------|
|    | ATOM | 4787 | CG1 | VAL | A | 598 | 5.739 | 48.974 | 69.142 | 1.00 | 15.98 |
|    | ATOM | 4788 | CG2 | VAL | A | 598 | 4.169 | 49.498 | 67.132 | 1.00 | 17.75 |
|    | ATOM | 4789 | N   | THR | A | 599 | 6.521 | 52.548 | 69.605 | 1.00 | 17.91 |
| 5  | ATOM | 4790 | CA  | THR | A | 599 | 7.370 | 53.125 | 70.636 | 1.00 | 20.42 |
|    | ATOM | 4791 | C   | THR | A | 599 | 6.544 | 53.965 | 71.615 | 1.00 | 25.40 |
|    | ATOM | 4792 | O   | THR | A | 599 | 6.683 | 53.931 | 72.848 | 1.00 | 18.93 |
|    | ATOM | 4793 | CB  | THR | A | 599 | 8.436 | 53.999 | 69.997 | 1.00 | 17.80 |
|    | ATOM | 4794 | OG1 | THR | A | 599 | 9.082 | 53.238 | 68.989 | 1.00 | 19.92 |
| 10 | ATOM | 4795 | CG2 | THR | A | 599 | 9.399 | 54.486 | 71.090 | 1.00 | 17.59 |
|    | ATOM | 4796 | N   | ALA | A | 600 | 5.657 | 54.749 | 71.018 | 1.00 | 18.73 |
|    | ATOM | 4797 | CA  | ALA | A | 600 | 4.798 | 55.590 | 71.796 | 1.00 | 17.65 |
|    | ATOM | 4798 | C   | ALA | A | 600 | 3.971 | 54.764 | 72.739 | 1.00 | 20.00 |
|    | ATOM | 4799 | O   | ALA | A | 600 | 3.867 | 55.053 | 73.932 | 1.00 | 21.50 |
| 15 | ATOM | 4800 | CB  | ALA | A | 600 | 3.869 | 56.344 | 70.879 | 1.00 | 19.26 |
|    | ATOM | 4801 | N   | MET | A | 601 | 3.344 | 53.731 | 72.218 | 1.00 | 17.31 |
|    | ATOM | 4802 | CA  | MET | A | 601 | 2.539 | 52.928 | 73.126 | 1.00 | 15.28 |
|    | ATOM | 4803 | C   | MET | A | 601 | 3.409 | 52.308 | 74.224 | 1.00 | 17.52 |
|    | ATOM | 4804 | O   | MET | A | 601 | 3.018 | 52.245 | 75.371 | 1.00 | 15.39 |
| 20 | ATOM | 4805 | CB  | MET | A | 601 | 1.761 | 51.815 | 72.369 | 1.00 | 16.44 |
|    | ATOM | 4806 | CG  | MET | A | 601 | 1.008 | 50.813 | 73.242 | 1.00 | 20.22 |
|    | ATOM | 4807 | SD  | MET | A | 601 | 1.962 | 49.492 | 74.103 | 1.00 | 24.22 |
|    | ATOM | 4808 | CE  | MET | A | 601 | 2.327 | 48.392 | 72.695 | 1.00 | 18.59 |
|    | ATOM | 4809 | N   | LEU | A | 602 | 4.580 | 51.778 | 73.889 | 1.00 | 16.21 |
| 25 | ATOM | 4810 | CA  | LEU | A | 602 | 5.389 | 51.117 | 74.924 | 1.00 | 16.19 |
|    | ATOM | 4811 | C   | LEU | A | 602 | 5.940 | 52.055 | 76.027 | 1.00 | 18.15 |
|    | ATOM | 4812 | O   | LEU | A | 602 | 5.962 | 51.722 | 77.214 | 1.00 | 18.36 |
|    | ATOM | 4813 | CB  | LEU | A | 602 | 6.507 | 50.267 | 74.269 | 1.00 | 14.21 |
|    | ATOM | 4814 | CG  | LEU | A | 602 | 5.987 | 49.058 | 73.508 | 1.00 | 18.02 |
| 30 | ATOM | 4815 | CD1 | LEU | A | 602 | 7.100 | 48.467 | 72.642 | 1.00 | 17.78 |
|    | ATOM | 4816 | CD2 | LEU | A | 602 | 5.502 | 48.030 | 74.515 | 1.00 | 21.84 |
|    | ATOM | 4817 | N   | VAL | A | 603 | 6.426 | 53.224 | 75.617 | 1.00 | 15.71 |
|    | ATOM | 4818 | CA  | VAL | A | 603 | 6.962 | 54.208 | 76.549 | 1.00 | 15.67 |
|    | ATOM | 4819 | C   | VAL | A | 603 | 5.877 | 54.648 | 77.537 | 1.00 | 17.35 |
| 35 | ATOM | 4820 | O   | VAL | A | 603 | 6.093 | 54.733 | 78.741 | 1.00 | 18.72 |
|    | ATOM | 4821 | CB  | VAL | A | 603 | 7.665 | 55.345 | 75.807 | 1.00 | 19.16 |
|    | ATOM | 4822 | CG1 | VAL | A | 603 | 8.035 | 56.477 | 76.764 | 1.00 | 15.61 |
|    | ATOM | 4823 | CG2 | VAL | A | 603 | 8.943 | 54.837 | 75.115 | 1.00 | 17.56 |
|    | ATOM | 4824 | N   | GLY | A | 604 | 4.661 | 54.851 | 77.027 | 1.00 | 14.92 |
| 40 | ATOM | 4825 | CA  | GLY | A | 604 | 3.535 | 55.262 | 77.879 | 1.00 | 14.02 |
|    | ATOM | 4826 | C   | GLY | A | 604 | 3.239 | 54.206 | 78.898 | 1.00 | 17.85 |
|    | ATOM | 4827 | O   | GLY | A | 604 | 2.984 | 54.443 | 80.075 | 1.00 | 21.21 |
|    | ATOM | 4828 | N   | LYS | A | 605 | 3.306 | 52.987 | 78.426 | 1.00 | 16.57 |
|    | ATOM | 4829 | CA  | LYS | A | 605 | 3.127 | 51.873 | 79.330 | 1.00 | 18.08 |
| 45 | ATOM | 4830 | C   | LYS | A | 605 | 4.251 | 51.892 | 80.348 | 1.00 | 22.76 |
|    | ATOM | 4831 | O   | LYS | A | 605 | 4.034 | 51.859 | 81.558 | 1.00 | 26.27 |
|    | ATOM | 4832 | CB  | LYS | A | 605 | 3.190 | 50.541 | 78.607 | 1.00 | 22.73 |
|    | ATOM | 4833 | CG  | LYS | A | 605 | 1.870 | 49.811 | 78.714 | 1.00 | 40.15 |
|    | ATOM | 4834 | CD  | LYS | A | 605 | 1.919 | 48.377 | 78.211 | 1.00 | 57.40 |
| 50 | ATOM | 4835 | CE  | LYS | A | 605 | 1.068 | 47.461 | 79.074 | 1.00 | 75.31 |
|    | ATOM | 4836 | NZ  | LYS | A | 605 | 1.808 | 46.387 | 79.758 | 1.00 | 74.64 |
|    | ATOM | 4837 | N   | ASP | A | 606 | 5.470 | 51.943 | 79.836 | 1.00 | 17.17 |
|    | ATOM | 4838 | CA  | ASP | A | 606 | 6.607 | 51.972 | 80.718 | 1.00 | 16.61 |
|    | ATOM | 4839 | C   | ASP | A | 606 | 6.442 | 53.059 | 81.738 | 1.00 | 19.46 |
| 55 | ATOM | 4840 | O   | ASP | A | 606 | 6.790 | 52.848 | 82.884 | 1.00 | 19.57 |
|    | ATOM | 4841 | CB  | ASP | A | 606 | 7.945 | 52.255 | 79.990 | 1.00 | 16.98 |
|    | ATOM | 4842 | CG  | ASP | A | 606 | 8.365 | 51.063 | 79.187 | 1.00 | 21.21 |
|    | ATOM | 4843 | OD1 | ASP | A | 606 | 7.944 | 49.933 | 79.376 | 1.00 | 20.21 |
|    | ATOM | 4844 | OD2 | ASP | A | 606 | 9.189 | 51.355 | 78.249 | 1.00 | 18.07 |
| 60 | ATOM | 4845 | N   | LEU | A | 607 | 5.974 | 54.207 | 81.306 | 1.00 | 16.61 |
|    | ATOM | 4846 | CA  | LEU | A | 607 | 5.863 | 55.352 | 82.211 | 1.00 | 20.64 |
|    | ATOM | 4847 | C   | LEU | A | 607 | 4.586 | 55.384 | 83.026 | 1.00 | 27.05 |
|    | ATOM | 4848 | O   | LEU | A | 607 | 4.361 | 56.274 | 83.862 | 1.00 | 23.83 |
|    | ATOM | 4849 | CB  | LEU | A | 607 | 5.991 | 56.641 | 81.388 | 1.00 | 23.11 |
|    | ATOM | 4850 | CG  | LEU | A | 607 | 7.377 | 57.301 | 81.464 | 1.00 | 28.84 |



|    |      |      |      |     |   |     |         |        |        |      |        |
|----|------|------|------|-----|---|-----|---------|--------|--------|------|--------|
|    | ATOM | 4851 | CD1  | LEU | A | 607 | 8.508   | 56.323 | 81.711 | 1.00 | 29.33  |
|    | ATOM | 4852 | CD2  | LEU | A | 607 | 7.650   | 58.116 | 80.214 | 1.00 | 19.22  |
|    | ATOM | 4853 | N    | LYS | A | 608 | 3.739   | 54.409 | 82.739 | 1.00 | 21.45  |
| 5  | ATOM | 4854 | CA   | LYS | A | 608 | 2.504   | 54.308 | 83.446 | 1.00 | 22.51  |
|    | ATOM | 4855 | C    | LYS | A | 608 | 1.657   | 55.529 | 83.202 | 1.00 | 31.79  |
|    | ATOM | 4856 | O    | LYS | A | 608 | 0.933   | 56.008 | 84.076 | 1.00 | 34.10  |
|    | ATOM | 4857 | CB   | LYS | A | 608 | 2.810   | 54.200 | 84.918 | 1.00 | 24.85  |
|    | ATOM | 4858 | CG   | LYS | A | 608 | 3.190   | 52.782 | 85.308 | 1.00 | 45.51  |
| 10 | ATOM | 4859 | CD   | LYS | A | 608 | 3.932   | 52.718 | 86.635 | 1.00 | 76.45  |
|    | ATOM | 4860 | CE   | LYS | A | 608 | 4.251   | 51.291 | 87.078 | 1.00 | 100.00 |
|    | ATOM | 4861 | NZ   | LYS | A | 608 | 4.137   | 51.050 | 88.533 | 1.00 | 100.00 |
|    | ATOM | 4862 | N    | VAL | A | 609 | 1.781   | 56.084 | 82.021 | 1.00 | 29.53  |
|    | ATOM | 4863 | CA   | VAL | A | 609 | 0.962   | 57.231 | 81.738 | 1.00 | 32.22  |
| 15 | ATOM | 4864 | C    | VAL | A | 609 | -0.257  | 56.755 | 80.958 | 1.00 | 47.38  |
|    | ATOM | 4865 | O    | VAL | A | 609 | -0.150  | 55.800 | 80.186 | 1.00 | 49.22  |
|    | ATOM | 4866 | CB   | VAL | A | 609 | 1.679   | 58.328 | 80.966 | 1.00 | 38.27  |
|    | ATOM | 4867 | CG1  | VAL | A | 609 | 3.188   | 58.240 | 81.067 | 1.00 | 38.12  |
|    | ATOM | 4868 | CG2  | VAL | A | 609 | 1.227   | 58.313 | 79.515 | 1.00 | 39.79  |
| 20 | ATOM | 4869 | N    | ASP | A | 610 | -1.402  | 57.415 | 81.173 | 1.00 | 49.29  |
|    | ATOM | 4870 | CA   | ASP | A | 610 | -2.675  | 57.124 | 80.510 | 1.00 | 98.66  |
|    | ATOM | 4871 | C    | ASP | A | 610 | -3.541  | 56.207 | 81.365 | 1.00 | 100.00 |
|    | ATOM | 4872 | O    | ASP | A | 610 | -3.950  | 56.568 | 82.470 | 1.00 | 78.31  |
|    | ATOM | 4873 | CB   | ASP | A | 610 | -2.550  | 56.631 | 79.044 | 1.00 | 100.00 |
| 25 | ATOM | 4874 | CG   | ASP | A | 610 | -1.930  | 57.631 | 78.091 | 1.00 | 100.00 |
|    | ATOM | 4875 | OD1  | ASP | A | 610 | -2.251  | 58.807 | 78.062 | 1.00 | 99.48  |
|    | ATOM | 4876 | OD2  | ASP | A | 610 | -1.019  | 57.111 | 77.288 | 1.00 | 100.00 |
|    | TER  | 4877 |      | ASP | A | 610 |         |        |        |      |        |
|    | ATOM | 4878 | ZN2+ | ZN  | Z | 1   | 16.972  | 39.340 | 64.102 | 1.00 | 16.33  |
| 30 | ATOM | 4879 | YB3+ | YB  | Y | 1   | 42.669  | 51.366 | 99.201 | 1.00 | 18.06  |
|    | ATOM | 4880 | YB3+ | YB  | Y | 2   | -13.732 | 57.497 | 52.155 | 0.50 | 46.53  |
|    | ATOM | 4881 | YB3+ | YB  | Y | 3   | -10.443 | 58.443 | 52.469 | 0.50 | 30.25  |
|    | ATOM | 4882 | N2   | BES | B | 1   | 13.712  | 41.186 | 63.145 | 1.00 | 25.72  |
|    | ATOM | 4883 | C1   | BES | B | 1   | 14.450  | 41.733 | 64.255 | 1.00 | 24.13  |
| 35 | ATOM | 4884 | C6   | BES | B | 1   | 13.749  | 42.939 | 64.880 | 1.00 | 23.84  |
|    | ATOM | 4885 | C7   | BES | B | 1   | 12.300  | 42.727 | 65.283 | 1.00 | 19.51  |
|    | ATOM | 4886 | C8   | BES | B | 1   | 11.297  | 43.571 | 64.799 | 1.00 | 18.42  |
|    | ATOM | 4887 | C12  | BES | B | 1   | 11.934  | 41.717 | 66.170 | 1.00 | 19.27  |
|    | ATOM | 4888 | C9   | BES | B | 1   | 9.990   | 43.454 | 65.227 | 1.00 | 16.90  |
| 40 | ATOM | 4889 | C11  | BES | B | 1   | 10.614  | 41.580 | 66.600 | 1.00 | 19.17  |
|    | ATOM | 4890 | C10  | BES | B | 1   | 9.639   | 42.451 | 66.135 | 1.00 | 18.42  |
|    | ATOM | 4891 | C2   | BES | B | 1   | 15.881  | 42.065 | 63.795 | 1.00 | 21.80  |
|    | ATOM | 4892 | O2   | BES | B | 1   | 16.369  | 41.004 | 62.999 | 1.00 | 18.60  |
| 45 | ATOM | 4893 | C3   | BES | B | 1   | 16.741  | 42.156 | 65.063 | 1.00 | 23.33  |
|    | ATOM | 4894 | O3   | BES | B | 1   | 16.932  | 41.185 | 65.803 | 1.00 | 25.68  |
|    | ATOM | 4895 | N1   | BES | B | 1   | 17.280  | 43.376 | 65.250 | 1.00 | 21.90  |
|    | ATOM | 4896 | C4   | BES | B | 1   | 18.157  | 43.613 | 66.390 | 1.00 | 24.18  |
|    | ATOM | 4897 | C13  | BES | B | 1   | 19.568  | 43.595 | 65.855 | 1.00 | 22.49  |
|    | ATOM | 4898 | C14  | BES | B | 1   | 20.669  | 42.812 | 66.576 | 1.00 | 24.23  |
| 50 | ATOM | 4899 | C15  | BES | B | 1   | 20.210  | 41.770 | 67.577 | 1.00 | 23.32  |
|    | ATOM | 4900 | C16  | BES | B | 1   | 21.692  | 42.287 | 65.590 | 1.00 | 22.52  |
|    | ATOM | 4901 | C5   | BES | B | 1   | 17.840  | 45.000 | 67.053 | 1.00 | 25.70  |
|    | ATOM | 4902 | O1   | BES | B | 1   | 17.160  | 45.848 | 66.348 | 1.00 | 22.63  |
|    | ATOM | 4903 | O4   | BES | B | 1   | 18.206  | 45.226 | 68.192 | 1.00 | 26.52  |
| 55 | ATOM | 4904 | CG   | IMD | I | 1   | 26.142  | 42.633 | 80.576 | 1.00 | 14.44  |
|    | ATOM | 4905 | ND1  | IMD | I | 1   | 25.962  | 42.811 | 79.218 | 1.00 | 15.15  |
|    | ATOM | 4906 | CD2  | IMD | I | 1   | 27.444  | 42.291 | 80.744 | 1.00 | 13.81  |
|    | ATOM | 4907 | CE1  | IMD | I | 1   | 27.096  | 42.555 | 78.588 | 1.00 | 9.17   |
|    | ATOM | 4908 | NE2  | IMD | I | 1   | 28.014  | 42.249 | 79.494 | 1.00 | 21.14  |
| 60 | ATOM | 4909 | CB   | ACE | C | 1   | 13.753  | 12.531 | 68.686 | 1.00 | 39.29  |
|    | ATOM | 4910 | CG   | ACE | C | 1   | 13.041  | 13.755 | 69.176 | 1.00 | 52.31  |
|    | ATOM | 4911 | OD1  | ACE | C | 1   | 13.310  | 14.951 | 68.885 | 1.00 | 21.34  |
|    | ATOM | 4912 | OD2  | ACE | C | 1   | 12.075  | 13.324 | 69.958 | 1.00 | 27.10  |
|    | ATOM | 4913 | O    | HOH | W | 1   | 23.792  | 34.258 | 75.188 | 1.00 | 13.41  |
|    | ATOM | 4914 | O    | HOH | W | 2   | 41.402  | 41.645 | 77.736 | 1.00 | 18.41  |



|    |      |      |   |     |   |    |        |        |        |      |        |
|----|------|------|---|-----|---|----|--------|--------|--------|------|--------|
|    | ATOM | 4915 | O | HOH | W | 3  | 21.452 | 48.008 | 79.289 | 1.00 | 14.29  |
|    | ATOM | 4916 | O | HOH | W | 4  | 7.395  | 22.508 | 68.980 | 1.00 | 15.42  |
|    | ATOM | 4917 | O | HOH | W | 5  | 8.875  | 45.610 | 71.521 | 1.00 | 15.01  |
| 5  | ATOM | 4918 | O | HOH | W | 6  | 18.318 | 15.775 | 81.560 | 1.00 | 42.99  |
|    | ATOM | 4919 | O | HOH | W | 7  | 30.607 | 45.406 | 73.230 | 1.00 | 16.49  |
|    | ATOM | 4920 | O | HOH | W | 8  | 2.151  | 35.326 | 56.132 | 1.00 | 20.69  |
|    | ATOM | 4921 | O | HOH | W | 9  | 26.371 | 45.237 | 72.729 | 1.00 | 32.21  |
|    | ATOM | 4922 | O | HOH | W | 10 | 10.117 | 47.411 | 58.465 | 1.00 | 19.66  |
| 10 | ATOM | 4923 | O | HOH | W | 11 | 24.576 | 45.901 | 81.764 | 1.00 | 15.98  |
|    | ATOM | 4924 | O | HOH | W | 12 | 21.400 | 39.522 | 70.350 | 1.00 | 17.59  |
|    | ATOM | 4925 | O | HOH | W | 13 | 32.755 | 39.688 | 76.763 | 1.00 | 14.73  |
|    | ATOM | 4926 | O | HOH | W | 14 | 15.723 | 43.292 | 73.593 | 1.00 | 28.15  |
|    | ATOM | 4927 | O | HOH | W | 15 | 33.012 | 53.990 | 68.029 | 1.00 | 20.61  |
| 15 | ATOM | 4928 | O | HOH | W | 16 | 21.672 | 48.368 | 86.318 | 1.00 | 18.35  |
|    | ATOM | 4929 | O | HOH | W | 17 | 11.843 | 66.293 | 86.775 | 1.00 | 20.28  |
|    | ATOM | 4930 | O | HOH | W | 18 | -7.370 | 39.258 | 72.858 | 1.00 | 100.00 |
|    | ATOM | 4931 | O | HOH | W | 19 | 10.951 | 58.853 | 90.712 | 1.00 | 31.18  |
|    | ATOM | 4932 | O | HOH | W | 20 | 7.991  | 67.991 | 69.688 | 1.00 | 51.29  |
| 20 | ATOM | 4933 | O | HOH | W | 21 | 27.534 | 25.933 | 83.686 | 1.00 | 30.42  |
|    | ATOM | 4934 | O | HOH | W | 22 | 14.754 | 47.886 | 81.192 | 1.00 | 91.59  |
|    | ATOM | 4935 | O | HOH | W | 23 | 35.638 | 66.681 | 74.616 | 1.00 | 18.43  |
|    | ATOM | 4936 | O | HOH | W | 24 | 14.917 | 46.651 | 71.292 | 1.00 | 29.09  |
|    | ATOM | 4937 | O | HOH | W | 25 | 24.339 | 72.545 | 82.858 | 1.00 | 27.38  |
| 25 | ATOM | 4938 | O | HOH | W | 26 | 3.954  | 59.653 | 64.218 | 1.00 | 29.75  |
|    | ATOM | 4939 | O | HOH | W | 27 | 0.174  | 30.326 | 72.099 | 1.00 | 20.53  |
|    | ATOM | 4940 | O | HOH | W | 28 | 17.250 | 55.520 | 87.251 | 1.00 | 15.14  |
|    | ATOM | 4941 | O | HOH | W | 29 | 2.640  | 38.007 | 61.525 | 1.00 | 15.01  |
|    | ATOM | 4942 | O | HOH | W | 30 | 10.861 | 36.115 | 89.266 | 1.00 | 26.76  |
| 30 | ATOM | 4943 | O | HOH | W | 31 | 30.988 | 44.243 | 70.800 | 1.00 | 37.98  |
|    | ATOM | 4944 | O | HOH | W | 32 | 9.095  | 44.675 | 75.314 | 1.00 | 24.97  |
|    | ATOM | 4945 | O | HOH | W | 33 | 29.917 | 47.569 | 70.312 | 1.00 | 33.43  |
|    | ATOM | 4946 | O | HOH | W | 34 | 23.537 | 45.186 | 73.070 | 1.00 | 21.89  |
|    | ATOM | 4947 | O | HOH | W | 35 | 13.919 | 30.086 | 87.520 | 1.00 | 27.60  |
| 35 | ATOM | 4948 | O | HOH | W | 36 | 24.004 | 28.230 | 84.950 | 1.00 | 54.91  |
|    | ATOM | 4949 | O | HOH | W | 37 | 44.740 | 56.907 | 93.797 | 1.00 | 39.70  |
|    | ATOM | 4950 | O | HOH | W | 38 | 36.453 | 36.919 | 75.700 | 1.00 | 12.06  |
|    | ATOM | 4951 | O | HOH | W | 39 | 27.587 | 65.302 | 75.920 | 1.00 | 21.02  |
|    | ATOM | 4952 | O | HOH | W | 40 | 23.077 | 39.811 | 87.155 | 1.00 | 38.48  |
| 40 | ATOM | 4953 | O | HOH | W | 41 | 3.661  | 37.055 | 59.039 | 1.00 | 17.86  |
|    | ATOM | 4954 | O | HOH | W | 42 | 21.794 | 20.673 | 79.219 | 1.00 | 20.60  |
|    | ATOM | 4955 | O | HOH | W | 43 | 6.324  | 36.055 | 87.167 | 1.00 | 30.35  |
|    | ATOM | 4956 | O | HOH | W | 44 | 24.649 | 34.194 | 44.975 | 1.00 | 52.51  |
|    | ATOM | 4957 | O | HOH | W | 45 | 20.611 | 44.717 | 78.685 | 1.00 | 27.41  |
| 45 | ATOM | 4958 | O | HOH | W | 46 | 19.969 | 50.884 | 89.461 | 1.00 | 29.62  |
|    | ATOM | 4959 | O | HOH | W | 47 | 30.940 | 66.808 | 78.811 | 1.00 | 15.76  |
|    | ATOM | 4960 | O | HOH | W | 48 | 26.539 | 55.260 | 66.886 | 1.00 | 19.97  |
|    | ATOM | 4961 | O | HOH | W | 49 | 7.314  | 45.436 | 77.867 | 1.00 | 35.07  |
|    | ATOM | 4962 | O | HOH | W | 50 | 10.579 | 54.800 | 67.603 | 1.00 | 15.62  |
| 50 | ATOM | 4963 | O | HOH | W | 51 | 28.138 | 31.371 | 66.611 | 1.00 | 15.08  |
|    | ATOM | 4964 | O | HOH | W | 52 | 26.292 | 33.348 | 75.129 | 1.00 | 15.49  |
|    | ATOM | 4965 | O | HOH | W | 53 | 15.204 | 48.508 | 69.331 | 1.00 | 16.03  |
|    | ATOM | 4966 | O | HOH | W | 54 | 9.451  | 57.282 | 68.158 | 1.00 | 20.39  |
|    | ATOM | 4967 | O | HOH | W | 55 | 34.923 | 67.738 | 77.001 | 1.00 | 15.06  |
| 55 | ATOM | 4968 | O | HOH | W | 56 | 10.193 | 53.763 | 78.443 | 1.00 | 19.23  |
|    | ATOM | 4969 | O | HOH | W | 57 | 35.246 | 32.562 | 64.227 | 1.00 | 27.89  |
|    | ATOM | 4970 | O | HOH | W | 58 | 7.230  | 48.517 | 65.509 | 1.00 | 17.57  |
|    | ATOM | 4971 | O | HOH | W | 59 | 15.707 | 29.269 | 62.146 | 1.00 | 16.76  |
|    | ATOM | 4972 | O | HOH | W | 60 | 22.703 | 46.209 | 83.610 | 1.00 | 14.72  |
| 60 | ATOM | 4973 | O | HOH | W | 61 | -5.573 | 31.742 | 67.048 | 1.00 | 67.53  |
|    | ATOM | 4974 | O | HOH | W | 62 | 23.958 | 46.448 | 79.118 | 1.00 | 14.95  |
|    | ATOM | 4975 | O | HOH | W | 63 | -4.387 | 51.289 | 59.224 | 1.00 | 29.13  |
|    | ATOM | 4976 | O | HOH | W | 64 | 1.494  | 43.916 | 68.255 | 1.00 | 21.32  |
|    | ATOM | 4977 | O | HOH | W | 65 | 15.236 | 37.185 | 89.202 | 1.00 | 24.71  |
|    | ATOM | 4978 | O | HOH | W | 66 | 8.901  | 44.256 | 58.842 | 1.00 | 22.41  |



|    |      |      |   |     |   |     |        |        |        |      |       |
|----|------|------|---|-----|---|-----|--------|--------|--------|------|-------|
|    | ATOM | 4979 | O | HOH | W | 67  | 8.741  | 44.059 | 69.410 | 1.00 | 19.23 |
|    | ATOM | 4980 | O | HOH | W | 68  | 10.536 | 31.361 | 71.130 | 1.00 | 17.26 |
|    | ATOM | 4981 | O | HOH | W | 69  | 14.270 | 66.977 | 85.494 | 1.00 | 24.71 |
| 5  | ATOM | 4982 | O | HOH | W | 70  | 19.324 | 33.013 | 51.120 | 1.00 | 31.37 |
|    | ATOM | 4983 | O | HOH | W | 71  | 22.888 | 42.589 | 71.900 | 1.00 | 32.53 |
|    | ATOM | 4984 | O | HOH | W | 72  | 18.199 | 19.792 | 50.850 | 1.00 | 95.99 |
|    | ATOM | 4985 | O | HOH | W | 73  | -2.766 | 36.708 | 53.654 | 1.00 | 25.61 |
|    | ATOM | 4986 | O | HOH | W | 74  | 40.154 | 44.352 | 89.098 | 1.00 | 18.04 |
|    | ATOM | 4987 | O | HOH | W | 75  | 43.798 | 45.414 | 76.216 | 1.00 | 42.09 |
| 10 | ATOM | 4988 | O | HOH | W | 76  | 2.095  | 33.636 | 67.241 | 1.00 | 16.77 |
|    | ATOM | 4989 | O | HOH | W | 77  | 17.697 | 47.834 | 68.674 | 1.00 | 15.55 |
|    | ATOM | 4990 | O | HOH | W | 78  | 0.487  | 49.526 | 68.994 | 1.00 | 40.71 |
|    | ATOM | 4991 | O | HOH | W | 79  | 24.958 | 57.027 | 93.315 | 1.00 | 15.83 |
|    | ATOM | 4992 | O | HOH | W | 80  | 16.157 | 27.572 | 83.036 | 1.00 | 20.90 |
| 15 | ATOM | 4993 | O | HOH | W | 81  | 5.222  | 49.330 | 63.415 | 1.00 | 17.36 |
|    | ATOM | 4994 | O | HOH | W | 82  | 16.211 | 37.941 | 52.836 | 1.00 | 19.88 |
|    | ATOM | 4995 | O | HOH | W | 83  | 32.789 | 43.179 | 86.654 | 1.00 | 20.34 |
|    | ATOM | 4996 | O | HOH | W | 84  | 9.298  | 48.075 | 81.153 | 1.00 | 54.83 |
|    | ATOM | 4997 | O | HOH | W | 85  | 29.454 | 36.152 | 82.527 | 1.00 | 29.31 |
| 20 | ATOM | 4998 | O | HOH | W | 86  | 41.926 | 50.859 | 91.024 | 1.00 | 26.91 |
|    | ATOM | 4999 | O | HOH | W | 87  | 42.353 | 47.486 | 84.905 | 1.00 | 21.77 |
|    | ATOM | 5000 | O | HOH | W | 88  | 7.099  | 45.738 | 66.261 | 1.00 | 16.80 |
|    | ATOM | 5001 | O | HOH | W | 89  | -7.189 | 40.950 | 62.864 | 1.00 | 18.87 |
|    | ATOM | 5002 | O | HOH | W | 90  | -0.532 | 35.957 | 55.006 | 1.00 | 30.96 |
| 25 | ATOM | 5003 | O | HOH | W | 91  | 2.498  | 58.239 | 62.223 | 1.00 | 33.64 |
|    | ATOM | 5004 | O | HOH | W | 92  | 8.030  | 54.347 | 85.172 | 1.00 | 36.67 |
|    | ATOM | 5005 | O | HOH | W | 93  | -9.086 | 47.257 | 64.010 | 1.00 | 25.14 |
|    | ATOM | 5006 | O | HOH | W | 94  | 7.634  | 23.157 | 71.565 | 1.00 | 26.48 |
|    | ATOM | 5007 | O | HOH | W | 95  | 36.802 | 57.687 | 75.942 | 1.00 | 33.51 |
| 30 | ATOM | 5008 | O | HOH | W | 96  | 31.266 | 28.847 | 81.561 | 1.00 | 33.78 |
|    | ATOM | 5009 | O | HOH | W | 97  | 42.718 | 53.265 | 90.455 | 1.00 | 18.15 |
|    | ATOM | 5010 | O | HOH | W | 98  | 25.175 | 49.362 | 94.064 | 1.00 | 38.55 |
|    | ATOM | 5011 | O | HOH | W | 99  | -1.458 | 36.897 | 71.377 | 1.00 | 21.47 |
|    | ATOM | 5012 | O | HOH | W | 100 | 36.955 | 22.462 | 67.101 | 1.00 | 62.30 |
| 35 | ATOM | 5013 | O | HOH | W | 101 | 17.777 | 47.785 | 75.841 | 1.00 | 20.17 |
|    | ATOM | 5014 | O | HOH | W | 102 | 17.194 | 41.841 | 54.112 | 1.00 | 16.39 |
|    | ATOM | 5015 | O | HOH | W | 103 | -1.972 | 55.370 | 57.254 | 1.00 | 25.11 |
|    | ATOM | 5016 | O | HOH | W | 104 | 27.602 | 40.677 | 72.586 | 1.00 | 21.30 |
|    | ATOM | 5017 | O | HOH | W | 105 | 37.435 | 51.467 | 61.104 | 1.00 | 65.38 |
| 40 | ATOM | 5018 | O | HOH | W | 106 | 1.256  | 32.447 | 69.628 | 1.00 | 23.44 |
|    | ATOM | 5019 | O | HOH | W | 107 | 9.241  | 16.192 | 63.327 | 1.00 | 48.00 |
|    | ATOM | 5020 | O | HOH | W | 108 | 0.854  | 36.054 | 64.035 | 1.00 | 18.60 |
|    | ATOM | 5021 | O | HOH | W | 109 | 18.727 | 44.131 | 84.651 | 1.00 | 24.89 |
|    | ATOM | 5022 | O | HOH | W | 110 | 26.098 | 18.961 | 78.803 | 1.00 | 24.48 |
| 45 | ATOM | 5023 | O | HOH | W | 111 | 19.158 | 42.699 | 78.273 | 1.00 | 28.07 |
|    | ATOM | 5024 | O | HOH | W | 112 | 38.525 | 39.961 | 90.164 | 1.00 | 49.63 |
|    | ATOM | 5025 | O | HOH | W | 113 | 18.603 | 45.487 | 82.264 | 1.00 | 21.64 |
|    | ATOM | 5026 | O | HOH | W | 114 | -9.935 | 47.106 | 60.568 | 1.00 | 27.24 |
|    | ATOM | 5027 | O | HOH | W | 115 | 12.837 | 36.710 | 59.433 | 1.00 | 15.13 |
| 50 | ATOM | 5028 | O | HOH | W | 116 | 33.438 | 65.032 | 85.997 | 1.00 | 32.21 |
|    | ATOM | 5029 | O | HOH | W | 117 | 38.122 | 36.535 | 73.494 | 1.00 | 12.50 |
|    | ATOM | 5030 | O | HOH | W | 118 | 39.258 | 66.537 | 78.047 | 1.00 | 18.65 |
|    | ATOM | 5031 | O | HOH | W | 119 | 6.554  | 34.671 | 88.987 | 1.00 | 15.86 |
|    | ATOM | 5032 | O | HOH | W | 120 | 13.095 | 46.874 | 73.346 | 1.00 | 30.35 |
| 55 | ATOM | 5033 | O | HOH | W | 121 | 32.660 | 36.335 | 82.732 | 1.00 | 35.47 |
|    | ATOM | 5034 | O | HOH | W | 122 | 9.605  | 28.610 | 88.505 | 1.00 | 19.15 |
|    | ATOM | 5035 | O | HOH | W | 123 | 27.330 | 46.500 | 69.982 | 1.00 | 28.22 |
|    | ATOM | 5036 | O | HOH | W | 124 | 21.495 | 44.397 | 85.333 | 1.00 | 27.70 |
|    | ATOM | 5037 | O | HOH | W | 125 | 25.964 | 67.884 | 90.313 | 1.00 | 24.59 |
| 60 | ATOM | 5038 | O | HOH | W | 126 | 39.654 | 61.279 | 78.612 | 1.00 | 34.08 |
|    | ATOM | 5039 | O | HOH | W | 127 | 28.830 | 50.839 | 62.528 | 1.00 | 22.84 |
|    | ATOM | 5040 | O | HOH | W | 128 | -2.192 | 25.904 | 60.928 | 1.00 | 48.99 |
|    | ATOM | 5041 | O | HOH | W | 129 | 12.941 | 37.733 | 62.998 | 1.00 | 17.09 |
|    | ATOM | 5042 | O | HOH | W | 130 | 17.656 | 39.494 | 55.302 | 1.00 | 23.77 |



|    |      |      |   |     |   |     |         |        |        |      |       |
|----|------|------|---|-----|---|-----|---------|--------|--------|------|-------|
|    | ATOM | 5043 | O | HOH | W | 131 | 5.616   | 31.767 | 78.251 | 1.00 | 22.11 |
|    | ATOM | 5044 | O | HOH | W | 132 | 11.134  | 59.317 | 68.286 | 1.00 | 24.37 |
|    | ATOM | 5045 | O | HOH | W | 133 | 7.669   | 46.689 | 57.186 | 1.00 | 19.15 |
| 5  | ATOM | 5046 | O | HOH | W | 134 | 24.475  | 34.718 | 86.839 | 1.00 | 32.19 |
|    | ATOM | 5047 | O | HOH | W | 135 | 23.517  | 44.933 | 68.463 | 1.00 | 20.25 |
|    | ATOM | 5048 | O | HOH | W | 136 | 26.942  | 39.752 | 68.390 | 1.00 | 15.96 |
|    | ATOM | 5049 | O | HOH | W | 137 | 8.029   | 20.133 | 84.468 | 1.00 | 16.28 |
|    | ATOM | 5050 | O | HOH | W | 138 | -0.771  | 45.529 | 78.260 | 1.00 | 68.55 |
| 10 | ATOM | 5051 | O | HOH | W | 139 | 44.023  | 49.889 | 77.980 | 1.00 | 30.04 |
|    | ATOM | 5052 | O | HOH | W | 140 | 26.786  | 62.061 | 81.604 | 1.00 | 16.85 |
|    | ATOM | 5053 | O | HOH | W | 141 | 13.879  | 47.676 | 76.209 | 1.00 | 46.91 |
|    | ATOM | 5054 | O | HOH | W | 142 | 25.840  | 58.036 | 65.771 | 1.00 | 54.37 |
|    | ATOM | 5055 | O | HOH | W | 143 | 10.922  | 53.966 | 85.792 | 1.00 | 18.98 |
| 15 | ATOM | 5056 | O | HOH | W | 144 | -12.182 | 45.374 | 45.449 | 1.00 | 33.96 |
|    | ATOM | 5057 | O | HOH | W | 145 | 31.206  | 39.579 | 79.369 | 1.00 | 15.60 |
|    | ATOM | 5058 | O | HOH | W | 146 | 15.440  | 42.222 | 77.590 | 1.00 | 25.43 |
|    | ATOM | 5059 | O | HOH | W | 147 | 0.824   | 56.052 | 62.386 | 1.00 | 26.41 |
|    | ATOM | 5060 | O | HOH | W | 148 | 44.978  | 53.578 | 86.262 | 1.00 | 22.60 |
| 20 | ATOM | 5061 | O | HOH | W | 149 | 17.898  | 31.967 | 86.834 | 1.00 | 19.51 |
|    | ATOM | 5062 | O | HOH | W | 150 | 15.892  | 63.944 | 61.374 | 1.00 | 54.27 |
|    | ATOM | 5063 | O | HOH | W | 151 | 29.311  | 44.330 | 75.316 | 1.00 | 39.02 |
|    | ATOM | 5064 | O | HOH | W | 152 | 11.678  | 62.566 | 52.561 | 1.00 | 27.61 |
|    | ATOM | 5065 | O | HOH | W | 153 | 26.748  | 53.479 | 95.785 | 1.00 | 45.53 |
| 25 | ATOM | 5066 | O | HOH | W | 154 | 35.164  | 39.157 | 88.454 | 1.00 | 33.28 |
|    | ATOM | 5067 | O | HOH | W | 155 | 13.599  | 30.411 | 61.539 | 1.00 | 16.55 |
|    | ATOM | 5068 | O | HOH | W | 156 | 2.955   | 41.496 | 60.167 | 1.00 | 26.41 |
|    | ATOM | 5069 | O | HOH | W | 157 | 21.013  | 47.058 | 81.902 | 1.00 | 24.07 |
|    | ATOM | 5070 | O | HOH | W | 158 | 7.082   | 15.804 | 68.963 | 1.00 | 13.64 |
| 30 | ATOM | 5071 | O | HOH | W | 159 | 43.659  | 51.565 | 97.228 | 1.00 | 13.91 |
|    | ATOM | 5072 | O | HOH | W | 160 | 25.728  | 46.521 | 67.857 | 1.00 | 15.18 |
|    | ATOM | 5073 | O | HOH | W | 161 | 16.336  | 27.429 | 80.519 | 1.00 | 13.58 |
|    | ATOM | 5074 | O | HOH | W | 162 | 13.506  | 27.963 | 78.488 | 1.00 | 11.63 |
|    | ATOM | 5075 | O | HOH | W | 163 | -1.826  | 28.836 | 60.633 | 1.00 | 18.21 |
| 35 | ATOM | 5076 | O | HOH | W | 164 | 2.041   | 28.523 | 68.718 | 1.00 | 19.80 |
|    | ATOM | 5077 | O | HOH | W | 165 | 39.832  | 50.082 | 92.567 | 1.00 | 15.76 |
|    | ATOM | 5078 | O | HOH | W | 166 | 20.417  | 35.797 | 44.686 | 1.00 | 23.98 |
|    | ATOM | 5079 | O | HOH | W | 167 | 36.272  | 60.259 | 74.993 | 1.00 | 26.08 |
|    | ATOM | 5080 | O | HOH | W | 168 | 5.426   | 61.205 | 63.338 | 1.00 | 23.06 |
| 40 | ATOM | 5081 | O | HOH | W | 169 | 17.667  | 67.608 | 77.116 | 1.00 | 28.66 |
|    | ATOM | 5082 | O | HOH | W | 170 | 5.631   | 18.160 | 69.508 | 1.00 | 19.48 |
|    | ATOM | 5083 | O | HOH | W | 171 | 22.328  | 62.979 | 93.415 | 1.00 | 25.81 |
|    | ATOM | 5084 | O | HOH | W | 172 | 40.390  | 48.175 | 94.855 | 1.00 | 47.37 |
|    | ATOM | 5085 | O | HOH | W | 173 | 17.444  | 40.095 | 51.789 | 1.00 | 18.19 |
| 45 | ATOM | 5086 | O | HOH | W | 174 | 29.587  | 24.011 | 76.681 | 1.00 | 24.09 |
|    | ATOM | 5087 | O | HOH | W | 175 | 6.778   | 26.010 | 80.637 | 1.00 | 26.64 |
|    | ATOM | 5088 | O | HOH | W | 176 | 43.821  | 42.250 | 81.895 | 1.00 | 24.88 |
|    | ATOM | 5089 | O | HOH | W | 177 | 28.198  | 18.300 | 60.474 | 1.00 | 24.14 |
|    | ATOM | 5090 | O | HOH | W | 178 | 22.788  | 46.771 | 90.209 | 1.00 | 24.26 |
|    | ATOM | 5091 | O | HOH | W | 179 | 29.931  | 24.564 | 79.534 | 1.00 | 31.74 |
| 50 | ATOM | 5092 | O | HOH | W | 180 | 10.739  | 18.587 | 70.209 | 1.00 | 34.82 |
|    | ATOM | 5093 | O | HOH | W | 181 | 3.737   | 42.980 | 66.727 | 1.00 | 18.45 |
|    | ATOM | 5094 | O | HOH | W | 182 | 10.657  | 69.135 | 86.850 | 1.00 | 30.21 |
|    | ATOM | 5095 | O | HOH | W | 183 | 23.612  | 39.959 | 68.861 | 1.00 | 20.99 |
| 55 | ATOM | 5096 | O | HOH | W | 184 | 30.240  | 50.378 | 93.511 | 1.00 | 31.76 |
|    | ATOM | 5097 | O | HOH | W | 185 | 24.407  | 42.363 | 69.680 | 1.00 | 23.63 |
|    | ATOM | 5098 | O | HOH | W | 186 | 3.121   | 26.698 | 57.992 | 1.00 | 26.26 |
|    | ATOM | 5099 | O | HOH | W | 187 | 6.662   | 51.993 | 60.872 | 1.00 | 21.24 |
|    | ATOM | 5100 | O | HOH | W | 188 | 10.549  | 31.727 | 52.631 | 1.00 | 21.12 |
|    | ATOM | 5101 | O | HOH | W | 189 | 7.213   | 14.560 | 66.229 | 1.00 | 19.68 |
| 60 | ATOM | 5102 | O | HOH | W | 190 | 10.944  | 37.995 | 74.849 | 1.00 | 26.21 |
|    | ATOM | 5103 | O | HOH | W | 191 | 29.009  | 38.268 | 80.361 | 1.00 | 21.40 |
|    | ATOM | 5104 | O | HOH | W | 192 | 8.720   | 37.803 | 87.790 | 1.00 | 25.70 |
|    | ATOM | 5105 | O | HOH | W | 193 | 30.731  | 47.721 | 57.132 | 1.00 | 25.12 |
|    | ATOM | 5106 | O | HOH | W | 194 | 21.085  | 45.693 | 69.052 | 1.00 | 27.11 |



|    |      |      |   |     |       |        |        |        |      |       |
|----|------|------|---|-----|-------|--------|--------|--------|------|-------|
| 5  | ATOM | 5107 | O | HOH | W 195 | 37.609 | 50.318 | 68.349 | 1.00 | 33.12 |
|    | ATOM | 5108 | O | HOH | W 196 | -4.270 | 35.004 | 72.084 | 1.00 | 23.92 |
|    | ATOM | 5109 | O | HOH | W 197 | 38.619 | 67.647 | 73.848 | 1.00 | 28.81 |
|    | ATOM | 5110 | O | HOH | W 198 | 0.963  | 27.263 | 54.964 | 1.00 | 25.61 |
|    | ATOM | 5111 | O | HOH | W 199 | 32.881 | 53.350 | 97.969 | 1.00 | 72.92 |
| 10 | ATOM | 5112 | O | HOH | W 200 | 16.605 | 54.411 | 65.120 | 1.00 | 21.12 |
|    | ATOM | 5113 | O | HOH | W 201 | 19.780 | 53.463 | 90.814 | 1.00 | 25.04 |
|    | ATOM | 5114 | O | HOH | W 202 | -7.941 | 56.718 | 56.011 | 1.00 | 40.98 |
|    | ATOM | 5115 | O | HOH | W 203 | 8.373  | 35.496 | 71.320 | 1.00 | 34.46 |
|    | ATOM | 5116 | O | HOH | W 204 | 30.102 | 60.104 | 96.117 | 1.00 | 23.15 |
| 15 | ATOM | 5117 | O | HOH | W 205 | 28.927 | 39.455 | 66.453 | 1.00 | 21.12 |
|    | ATOM | 5118 | O | HOH | W 206 | 39.689 | 41.335 | 88.297 | 1.00 | 27.24 |
|    | ATOM | 5119 | O | HOH | W 207 | 33.916 | 37.626 | 52.438 | 1.00 | 33.19 |
|    | ATOM | 5120 | O | HOH | W 208 | 1.622  | 50.963 | 82.588 | 1.00 | 50.35 |
|    | ATOM | 5121 | O | HOH | W 209 | 16.333 | 60.146 | 56.900 | 1.00 | 29.60 |
| 20 | ATOM | 5122 | O | HOH | W 210 | 39.242 | 45.128 | 91.725 | 1.00 | 22.90 |
|    | ATOM | 5123 | O | HOH | W 211 | 14.399 | 30.418 | 45.430 | 1.00 | 34.78 |
|    | ATOM | 5124 | O | HOH | W 212 | 29.888 | 42.111 | 88.891 | 1.00 | 34.76 |
|    | ATOM | 5125 | O | HOH | W 213 | 18.346 | 26.212 | 50.297 | 1.00 | 44.21 |
|    | ATOM | 5126 | O | HOH | W 214 | 22.864 | 63.026 | 74.711 | 1.00 | 29.30 |
| 25 | ATOM | 5127 | O | HOH | W 215 | 20.113 | 37.220 | 85.926 | 1.00 | 24.06 |
|    | ATOM | 5128 | O | HOH | W 216 | 23.298 | 70.540 | 87.208 | 1.00 | 35.89 |
|    | ATOM | 5129 | O | HOH | W 217 | 26.970 | 41.872 | 69.933 | 1.00 | 28.60 |
|    | ATOM | 5130 | O | HOH | W 218 | -4.296 | 44.927 | 43.216 | 1.00 | 33.90 |
|    | ATOM | 5131 | O | HOH | W 219 | 12.321 | 60.082 | 62.828 | 1.00 | 28.33 |
| 30 | ATOM | 5132 | O | HOH | W 220 | 13.873 | 37.878 | 45.419 | 1.00 | 43.55 |
|    | ATOM | 5133 | O | HOH | W 221 | 30.748 | 40.180 | 83.791 | 1.00 | 37.04 |
|    | ATOM | 5134 | O | HOH | W 222 | 15.784 | 58.732 | 93.087 | 1.00 | 23.80 |
|    | ATOM | 5135 | O | HOH | W 223 | 35.311 | 18.767 | 63.462 | 1.00 | 49.24 |
|    | ATOM | 5136 | O | HOH | W 224 | -0.325 | 33.536 | 77.400 | 1.00 | 28.59 |
| 35 | ATOM | 5137 | O | HOH | W 225 | 9.312  | 60.280 | 65.861 | 1.00 | 37.85 |
|    | ATOM | 5138 | O | HOH | W 226 | 20.424 | 20.146 | 83.661 | 1.00 | 32.68 |
|    | ATOM | 5139 | O | HOH | W 227 | 10.879 | 65.256 | 88.761 | 1.00 | 28.17 |
|    | ATOM | 5140 | O | HOH | W 228 | 6.481  | 11.890 | 66.154 | 1.00 | 13.58 |
|    | ATOM | 5141 | O | HOH | W 229 | 11.493 | 12.304 | 65.667 | 1.00 | 31.38 |
| 40 | ATOM | 5142 | O | HOH | W 230 | 23.893 | 48.760 | 67.764 | 1.00 | 19.58 |
|    | ATOM | 5143 | O | HOH | W 231 | 11.826 | 33.465 | 74.498 | 1.00 | 16.87 |
|    | ATOM | 5144 | O | HOH | W 232 | 20.228 | 48.799 | 84.083 | 1.00 | 14.10 |
|    | ATOM | 5145 | O | HOH | W 233 | 8.333  | 25.989 | 83.238 | 1.00 | 20.03 |
|    | ATOM | 5146 | O | HOH | W 234 | 24.244 | 65.422 | 90.512 | 1.00 | 18.61 |
| 45 | ATOM | 5147 | O | HOH | W 235 | 29.682 | 43.395 | 86.674 | 1.00 | 29.99 |
|    | ATOM | 5148 | O | HOH | W 236 | 32.122 | 38.935 | 81.421 | 1.00 | 21.98 |
|    | ATOM | 5149 | O | HOH | W 237 | 38.098 | 44.260 | 70.626 | 1.00 | 23.18 |
|    | ATOM | 5150 | O | HOH | W 238 | 17.172 | 68.773 | 81.829 | 1.00 | 33.19 |
|    | ATOM | 5151 | O | HOH | W 239 | 22.056 | 41.676 | 85.707 | 1.00 | 27.98 |
| 50 | ATOM | 5152 | O | HOH | W 240 | 10.609 | 35.835 | 76.035 | 1.00 | 26.77 |
|    | ATOM | 5153 | O | HOH | W 241 | 5.895  | 48.362 | 80.563 | 1.00 | 35.27 |
|    | ATOM | 5154 | O | HOH | W 242 | 4.210  | 38.365 | 90.354 | 1.00 | 62.63 |
|    | ATOM | 5155 | O | HOH | W 243 | 27.505 | 26.048 | 57.570 | 1.00 | 34.59 |
|    | ATOM | 5156 | O | HOH | W 244 | 40.199 | 29.895 | 75.610 | 1.00 | 30.81 |
| 55 | ATOM | 5157 | O | HOH | W 245 | 41.069 | 35.070 | 67.073 | 1.00 | 25.75 |
|    | ATOM | 5158 | O | HOH | W 246 | 18.209 | 43.386 | 70.174 | 1.00 | 24.27 |
|    | ATOM | 5159 | O | HOH | W 247 | 22.994 | 40.780 | 73.297 | 1.00 | 35.20 |
|    | ATOM | 5160 | O | HOH | W 248 | 11.980 | 17.646 | 61.687 | 1.00 | 24.63 |
|    | ATOM | 5161 | O | HOH | W 249 | 17.092 | 44.230 | 71.974 | 1.00 | 27.55 |
| 60 | ATOM | 5162 | O | HOH | W 250 | 29.907 | 45.909 | 50.610 | 1.00 | 33.85 |
|    | ATOM | 5163 | O | HOH | W 251 | 25.337 | 41.587 | 74.020 | 1.00 | 31.92 |
|    | ATOM | 5164 | O | HOH | W 252 | 34.320 | 29.393 | 64.417 | 1.00 | 34.88 |
|    | ATOM | 5165 | O | HOH | W 253 | 16.366 | 57.688 | 55.311 | 1.00 | 30.35 |
|    | ATOM | 5166 | O | HOH | W 254 | 25.295 | 70.347 | 83.432 | 1.00 | 44.62 |
|    | ATOM | 5167 | O | HOH | W 255 | 28.780 | 44.083 | 69.312 | 1.00 | 38.06 |
|    | ATOM | 5168 | O | HOH | W 256 | 43.987 | 44.841 | 81.855 | 1.00 | 26.92 |
|    | ATOM | 5169 | O | HOH | W 257 | 10.694 | 22.780 | 82.399 | 1.00 | 40.18 |
|    | ATOM | 5170 | O | HOH | W 258 | 3.209  | 26.059 | 69.842 | 1.00 | 50.02 |



|    |      |      |   |     |   |     |         |        |        |      |       |
|----|------|------|---|-----|---|-----|---------|--------|--------|------|-------|
|    | ATOM | 5171 | O | HOH | W | 259 | 25.123  | 69.880 | 90.995 | 1.00 | 32.08 |
|    | ATOM | 5172 | O | HOH | W | 260 | 10.460  | 60.937 | 72.334 | 1.00 | 28.48 |
|    | ATOM | 5173 | O | HOH | W | 261 | 35.272  | 43.014 | 54.933 | 1.00 | 35.32 |
| 5  | ATOM | 5174 | O | HOH | W | 262 | 31.555  | 49.428 | 69.261 | 1.00 | 30.03 |
|    | ATOM | 5175 | O | HOH | W | 263 | 18.455  | 45.339 | 74.865 | 1.00 | 22.60 |
|    | ATOM | 5176 | O | HOH | W | 264 | 0.397   | 52.925 | 76.187 | 1.00 | 26.73 |
|    | ATOM | 5177 | O | HOH | W | 265 | 24.642  | 68.564 | 81.573 | 1.00 | 27.40 |
|    | ATOM | 5178 | O | HOH | W | 266 | 25.734  | 20.393 | 55.492 | 1.00 | 32.87 |
| 10 | ATOM | 5179 | O | HOH | W | 267 | 11.923  | 58.720 | 70.763 | 1.00 | 21.77 |
|    | ATOM | 5180 | O | HOH | W | 268 | 30.308  | 43.013 | 67.201 | 1.00 | 35.32 |
|    | ATOM | 5181 | O | HOH | W | 269 | 39.640  | 38.126 | 67.437 | 1.00 | 28.94 |
|    | ATOM | 5182 | O | HOH | W | 270 | 10.397  | 50.110 | 41.557 | 1.00 | 28.07 |
|    | ATOM | 5183 | O | HOH | W | 271 | 33.290  | 46.466 | 61.539 | 1.00 | 27.30 |
| 15 | ATOM | 5184 | O | HOH | W | 272 | 0.016   | 42.090 | 76.502 | 1.00 | 32.33 |
|    | ATOM | 5185 | O | HOH | W | 273 | 26.563  | 45.481 | 40.291 | 1.00 | 47.85 |
|    | ATOM | 5186 | O | HOH | W | 274 | 30.451  | 15.205 | 70.110 | 1.00 | 33.04 |
|    | ATOM | 5187 | O | HOH | W | 275 | 0.678   | 54.618 | 69.973 | 1.00 | 30.37 |
|    | ATOM | 5188 | O | HOH | W | 276 | 31.009  | 22.826 | 58.292 | 1.00 | 38.03 |
| 20 | ATOM | 5189 | O | HOH | W | 277 | 11.598  | 18.077 | 78.103 | 1.00 | 32.86 |
|    | ATOM | 5190 | O | HOH | W | 278 | 42.789  | 49.257 | 82.276 | 1.00 | 38.27 |
|    | ATOM | 5191 | O | HOH | W | 279 | 22.610  | 37.483 | 44.945 | 1.00 | 36.88 |
|    | ATOM | 5192 | O | HOH | W | 280 | 19.095  | 19.104 | 54.480 | 1.00 | 29.52 |
|    | ATOM | 5193 | O | HOH | W | 281 | -17.217 | 39.695 | 36.067 | 1.00 | 33.38 |
| 25 | ATOM | 5194 | O | HOH | W | 282 | 6.068   | 42.637 | 67.543 | 1.00 | 33.87 |
|    | ATOM | 5195 | O | HOH | W | 283 | 20.639  | 46.522 | 87.847 | 1.00 | 36.70 |
|    | ATOM | 5196 | O | HOH | W | 284 | -8.870  | 56.242 | 58.240 | 1.00 | 50.62 |
|    | ATOM | 5197 | O | HOH | W | 285 | 16.582  | 61.670 | 59.151 | 1.00 | 38.20 |
|    | ATOM | 5198 | O | HOH | W | 286 | 42.501  | 43.301 | 75.886 | 1.00 | 27.81 |
| 30 | ATOM | 5199 | O | HOH | W | 287 | 25.604  | 33.439 | 84.786 | 1.00 | 21.08 |
|    | ATOM | 5200 | O | HOH | W | 288 | 13.520  | 67.352 | 52.561 | 1.00 | 39.75 |
|    | ATOM | 5201 | O | HOH | W | 289 | 9.627   | 28.198 | 45.908 | 1.00 | 37.35 |
|    | ATOM | 5202 | O | HOH | W | 290 | 18.134  | 36.512 | 88.493 | 1.00 | 43.01 |
|    | ATOM | 5203 | O | HOH | W | 291 | 22.300  | 20.482 | 81.874 | 1.00 | 37.81 |
| 35 | ATOM | 5204 | O | HOH | W | 292 | 44.203  | 41.289 | 79.602 | 1.00 | 27.00 |
|    | ATOM | 5205 | O | HOH | W | 293 | 44.462  | 52.335 | 93.395 | 1.00 | 32.88 |
|    | ATOM | 5206 | O | HOH | W | 294 | -2.968  | 37.813 | 43.815 | 1.00 | 39.42 |
|    | ATOM | 5207 | O | HOH | W | 295 | 14.615  | 50.638 | 83.483 | 1.00 | 40.84 |
|    | ATOM | 5208 | O | HOH | W | 296 | 17.655  | 48.236 | 85.049 | 1.00 | 38.41 |
| 40 | ATOM | 5209 | O | HOH | W | 297 | 25.105  | 58.534 | 70.338 | 1.00 | 45.37 |
|    | ATOM | 5210 | O | HOH | W | 298 | 6.153   | 22.174 | 58.465 | 1.00 | 51.17 |
|    | ATOM | 5211 | O | HOH | W | 299 | 14.099  | 45.045 | 75.129 | 1.00 | 38.12 |
|    | ATOM | 5212 | O | HOH | W | 300 | 3.614   | 33.798 | 78.265 | 1.00 | 33.77 |
|    | ATOM | 5213 | O | HOH | W | 301 | 10.974  | 62.101 | 70.086 | 1.00 | 31.30 |
| 45 | ATOM | 5214 | O | HOH | W | 302 | 7.585   | 38.532 | 71.479 | 1.00 | 35.66 |
|    | ATOM | 5215 | O | HOH | W | 303 | 20.998  | 44.178 | 74.359 | 1.00 | 37.38 |
|    | ATOM | 5216 | O | HOH | W | 304 | 11.918  | 38.385 | 43.252 | 1.00 | 35.61 |
|    | ATOM | 5217 | O | HOH | W | 305 | 34.337  | 29.948 | 80.309 | 1.00 | 36.78 |
|    | ATOM | 5218 | O | HOH | W | 306 | 39.120  | 63.630 | 75.316 | 1.00 | 43.48 |
| 50 | ATOM | 5219 | O | HOH | W | 307 | 36.491  | 64.702 | 80.717 | 1.00 | 19.64 |
|    | ATOM | 5220 | O | HOH | W | 308 | -11.598 | 58.968 | 55.040 | 1.00 | 54.59 |
|    | ATOM | 5221 | O | HOH | W | 309 | 18.873  | 53.508 | 93.447 | 1.00 | 29.42 |
|    | ATOM | 5222 | O | HOH | W | 310 | 7.673   | 37.412 | 69.273 | 1.00 | 30.92 |
|    | ATOM | 5223 | O | HOH | W | 311 | 38.494  | 29.355 | 71.433 | 1.00 | 35.92 |
| 55 | ATOM | 5224 | O | HOH | W | 312 | 2.378   | 64.614 | 72.106 | 1.00 | 23.68 |
|    | ATOM | 5225 | O | HOH | W | 313 | 34.055  | 22.747 | 70.419 | 1.00 | 47.42 |
|    | ATOM | 5226 | O | HOH | W | 314 | 6.517   | 15.338 | 63.891 | 1.00 | 39.21 |
|    | ATOM | 5227 | O | HOH | W | 315 | 33.135  | 58.667 | 95.357 | 1.00 | 38.27 |
|    | ATOM | 5228 | O | HOH | W | 316 | 7.877   | 41.088 | 68.810 | 1.00 | 30.88 |
| 60 | ATOM | 5229 | O | HOH | W | 317 | 4.500   | 63.686 | 62.465 | 1.00 | 40.54 |
|    | ATOM | 5230 | O | HOH | W | 318 | 32.594  | 44.212 | 51.619 | 1.00 | 28.18 |
|    | ATOM | 5231 | O | HOH | W | 319 | 19.892  | 28.363 | 50.295 | 1.00 | 37.48 |
|    | ATOM | 5232 | O | HOH | W | 320 | 38.121  | 42.209 | 58.482 | 1.00 | 35.42 |
|    | ATOM | 5233 | O | HOH | W | 321 | 18.953  | 60.209 | 59.879 | 1.00 | 32.37 |
|    | ATOM | 5234 | O | HOH | W | 322 | -1.038  | 45.854 | 73.695 | 1.00 | 33.19 |



|    |      |      |   |     |   |     |         |        |        |      |       |
|----|------|------|---|-----|---|-----|---------|--------|--------|------|-------|
|    | ATOM | 5235 | O | HOH | W | 323 | -6.723  | 31.695 | 78.229 | 1.00 | 48.52 |
|    | ATOM | 5236 | O | HOH | W | 324 | 20.123  | 41.413 | 71.190 | 1.00 | 40.23 |
|    | ATOM | 5237 | O | HOH | W | 325 | 5.380   | 25.588 | 55.751 | 1.00 | 26.30 |
| 5  | ATOM | 5238 | O | HOH | W | 326 | -8.946  | 53.154 | 58.636 | 1.00 | 33.33 |
|    | ATOM | 5239 | O | HOH | W | 327 | 5.224   | 20.615 | 65.617 | 1.00 | 38.04 |
|    | ATOM | 5240 | O | HOH | W | 328 | -0.951  | 44.688 | 66.660 | 1.00 | 48.71 |
|    | ATOM | 5241 | O | HOH | W | 329 | 9.548   | 17.972 | 61.116 | 1.00 | 38.57 |
|    | ATOM | 5242 | O | HOH | W | 330 | 16.170  | 45.478 | 46.564 | 1.00 | 33.55 |
| 10 | ATOM | 5243 | O | HOH | W | 331 | 28.152  | 31.228 | 86.919 | 1.00 | 66.11 |
|    | ATOM | 5244 | O | HOH | W | 332 | -4.227  | 32.608 | 61.396 | 1.00 | 29.03 |
|    | ATOM | 5245 | O | HOH | W | 333 | 23.532  | 69.913 | 79.399 | 1.00 | 40.45 |
|    | ATOM | 5246 | O | HOH | W | 334 | 16.943  | 25.394 | 84.026 | 1.00 | 35.64 |
|    | ATOM | 5247 | O | HOH | W | 335 | -6.097  | 33.164 | 72.143 | 1.00 | 47.23 |
| 15 | ATOM | 5248 | O | HOH | W | 336 | 26.639  | 58.545 | 95.902 | 1.00 | 30.17 |
|    | ATOM | 5249 | O | HOH | W | 337 | 18.090  | 14.281 | 77.183 | 1.00 | 34.77 |
|    | ATOM | 5250 | O | HOH | W | 338 | 16.783  | 69.158 | 79.498 | 1.00 | 41.04 |
|    | ATOM | 5251 | O | HOH | W | 339 | 44.586  | 50.422 | 83.945 | 1.00 | 37.92 |
|    | ATOM | 5252 | O | HOH | W | 340 | 11.828  | 51.361 | 43.560 | 1.00 | 42.10 |
| 20 | ATOM | 5253 | O | HOH | W | 341 | 22.773  | 36.745 | 86.817 | 1.00 | 38.07 |
|    | ATOM | 5254 | O | HOH | W | 342 | 26.608  | 43.969 | 74.943 | 1.00 | 32.64 |
|    | ATOM | 5255 | O | HOH | W | 343 | 14.797  | 17.437 | 79.901 | 1.00 | 37.80 |
|    | ATOM | 5256 | O | HOH | W | 344 | 32.755  | 40.414 | 86.886 | 1.00 | 53.20 |
|    | ATOM | 5257 | O | HOH | W | 345 | 23.938  | 65.851 | 93.231 | 1.00 | 38.25 |
| 25 | ATOM | 5258 | O | HOH | W | 346 | 34.689  | 68.947 | 70.635 | 1.00 | 32.36 |
|    | ATOM | 5259 | O | HOH | W | 347 | 32.902  | 14.779 | 66.467 | 1.00 | 55.05 |
|    | ATOM | 5260 | O | HOH | W | 348 | -0.197  | 59.892 | 61.918 | 1.00 | 41.09 |
|    | ATOM | 5261 | O | HOH | W | 349 | 35.933  | 50.743 | 66.825 | 1.00 | 29.14 |
|    | ATOM | 5262 | O | HOH | W | 350 | 21.451  | 70.196 | 84.069 | 1.00 | 37.63 |
| 30 | ATOM | 5263 | O | HOH | W | 351 | 10.392  | 34.055 | 71.909 | 1.00 | 37.36 |
|    | ATOM | 5264 | O | HOH | W | 352 | 16.118  | 48.288 | 46.594 | 1.00 | 33.56 |
|    | ATOM | 5265 | O | HOH | W | 353 | 2.277   | 58.481 | 67.819 | 1.00 | 45.09 |
|    | ATOM | 5266 | O | HOH | W | 354 | -21.140 | 42.970 | 52.987 | 1.00 | 38.49 |
|    | ATOM | 5267 | O | HOH | W | 355 | 0.364   | 56.797 | 65.209 | 1.00 | 34.76 |
| 35 | ATOM | 5268 | O | HOH | W | 356 | 9.763   | 37.511 | 72.464 | 1.00 | 36.84 |
|    | ATOM | 5269 | O | HOH | W | 357 | -3.293  | 29.651 | 64.159 | 1.00 | 48.44 |
|    | ATOM | 5270 | O | HOH | W | 358 | 18.653  | 59.497 | 55.820 | 1.00 | 41.32 |
|    | ATOM | 5271 | O | HOH | W | 359 | 18.360  | 56.858 | 89.365 | 1.00 | 16.20 |
|    | ATOM | 5272 | O | HOH | W | 360 | 19.264  | 58.334 | 58.324 | 1.00 | 24.32 |
| 40 | ATOM | 5273 | O | HOH | W | 361 | 19.786  | 68.920 | 85.535 | 1.00 | 36.46 |
|    | ATOM | 5274 | O | HOH | W | 362 | 0.891   | 46.454 | 70.028 | 1.00 | 49.40 |
|    | ATOM | 5275 | O | HOH | W | 363 | 13.401  | 15.156 | 61.247 | 1.00 | 32.90 |
|    | ATOM | 5276 | O | HOH | W | 364 | 29.937  | 41.912 | 73.484 | 1.00 | 34.92 |
|    | ATOM | 5277 | O | HOH | W | 365 | 28.117  | 39.053 | 82.612 | 1.00 | 29.94 |
| 45 | ATOM | 5278 | O | HOH | W | 366 | 17.060  | 44.064 | 76.687 | 1.00 | 31.64 |
|    | ATOM | 5279 | O | HOH | W | 367 | 7.781   | 32.331 | 42.244 | 1.00 | 54.33 |
|    | ATOM | 5280 | O | HOH | W | 368 | 13.484  | 60.143 | 67.092 | 1.00 | 36.32 |
|    | ATOM | 5281 | O | HOH | W | 369 | 4.972   | 65.695 | 69.472 | 1.00 | 30.93 |
|    | ATOM | 5282 | O | HOH | W | 370 | 20.859  | 55.364 | 94.926 | 1.00 | 35.05 |
| 50 | ATOM | 5283 | O | HOH | W | 371 | 29.891  | 64.316 | 94.062 | 1.00 | 32.43 |
|    | ATOM | 5284 | O | HOH | W | 372 | 31.636  | 50.857 | 46.407 | 1.00 | 75.60 |
|    | ATOM | 5285 | O | HOH | W | 373 | -9.778  | 35.027 | 39.632 | 1.00 | 56.74 |
|    | ATOM | 5286 | O | HOH | W | 374 | 14.152  | 12.701 | 64.957 | 1.00 | 23.80 |
|    | ATOM | 5287 | O | HOH | W | 375 | 35.419  | 45.143 | 64.442 | 1.00 | 36.74 |
| 55 | ATOM | 5288 | O | HOH | W | 376 | 34.839  | 57.375 | 97.888 | 1.00 | 34.34 |
|    | ATOM | 5289 | O | HOH | W | 377 | 35.027  | 44.946 | 53.379 | 1.00 | 45.25 |
|    | ATOM | 5290 | O | HOH | W | 378 | 10.904  | 44.942 | 78.238 | 1.00 | 46.33 |
|    | ATOM | 5291 | O | HOH | W | 379 | 2.265   | 29.749 | 79.673 | 1.00 | 55.34 |
|    | ATOM | 5292 | O | HOH | W | 380 | 38.376  | 37.663 | 83.485 | 1.00 | 48.83 |
| 60 | ATOM | 5293 | O | HOH | W | 381 | 7.069   | 18.511 | 64.588 | 1.00 | 42.75 |
|    | ATOM | 5294 | O | HOH | W | 382 | 10.013  | 63.184 | 65.119 | 1.00 | 51.27 |
|    | ATOM | 5295 | O | HOH | W | 383 | 26.880  | 67.265 | 80.460 | 1.00 | 29.17 |
|    | ATOM | 5296 | O | HOH | W | 384 | 5.435   | 44.858 | 39.529 | 1.00 | 44.09 |
|    | ATOM | 5297 | O | HOH | W | 385 | 12.020  | 76.116 | 49.503 | 1.00 | 57.08 |
|    | ATOM | 5298 | O | HOH | W | 386 | 4.495   | 69.223 | 72.134 | 1.00 | 39.49 |



|    |      |      |   |     |   |     |         |        |        |      |       |
|----|------|------|---|-----|---|-----|---------|--------|--------|------|-------|
| 5  | ATOM | 5299 | O | HOH | W | 387 | 34.373  | 34.834 | 52.407 | 1.00 | 45.73 |
|    | ATOM | 5300 | O | HOH | W | 388 | -0.366  | 52.210 | 68.045 | 1.00 | 56.86 |
|    | ATOM | 5301 | O | HOH | W | 389 | 15.108  | 39.899 | 89.165 | 1.00 | 30.62 |
|    | ATOM | 5302 | O | HOH | W | 390 | 20.977  | 60.725 | 61.985 | 1.00 | 42.08 |
|    | ATOM | 5303 | O | HOH | W | 391 | 29.038  | 14.547 | 63.725 | 1.00 | 33.69 |
| 10 | ATOM | 5304 | O | HOH | W | 392 | 34.064  | 66.637 | 81.988 | 1.00 | 37.83 |
|    | ATOM | 5305 | O | HOH | W | 393 | 8.669   | 71.915 | 54.348 | 1.00 | 40.01 |
|    | ATOM | 5306 | O | HOH | W | 394 | 4.823   | 29.577 | 79.259 | 1.00 | 42.09 |
|    | ATOM | 5307 | O | HOH | W | 395 | 22.745  | 32.929 | 42.078 | 1.00 | 50.18 |
|    | ATOM | 5308 | O | HOH | W | 396 | 0.658   | 29.749 | 51.236 | 1.00 | 30.86 |
| 15 | ATOM | 5309 | O | HOH | W | 397 | 3.793   | 58.214 | 86.346 | 1.00 | 62.42 |
|    | ATOM | 5310 | O | HOH | W | 398 | 12.206  | 40.564 | 89.850 | 1.00 | 39.66 |
|    | ATOM | 5311 | O | HOH | W | 399 | 21.573  | 25.561 | 53.053 | 1.00 | 34.62 |
|    | ATOM | 5312 | O | HOH | W | 400 | 30.197  | 56.551 | 58.739 | 1.00 | 40.16 |
|    | ATOM | 5313 | O | HOH | W | 401 | 20.406  | 59.350 | 64.941 | 1.00 | 33.97 |
| 20 | ATOM | 5314 | O | HOH | W | 402 | 16.956  | 52.960 | 87.724 | 1.00 | 54.35 |
|    | ATOM | 5315 | O | HOH | W | 403 | 36.719  | 27.459 | 68.822 | 1.00 | 42.51 |
|    | ATOM | 5316 | O | HOH | W | 404 | 7.458   | 27.206 | 77.481 | 1.00 | 46.67 |
|    | ATOM | 5317 | O | HOH | W | 405 | 36.220  | 64.298 | 90.593 | 1.00 | 51.29 |
|    | ATOM | 5318 | O | HOH | W | 406 | -17.985 | 43.406 | 48.900 | 1.00 | 41.71 |
| 25 | ATOM | 5319 | O | HOH | W | 407 | 1.914   | 29.246 | 53.120 | 1.00 | 38.28 |
|    | ATOM | 5320 | O | HOH | W | 408 | -4.267  | 29.328 | 73.970 | 1.00 | 34.50 |
|    | ATOM | 5321 | O | HOH | W | 409 | 14.000  | 53.360 | 42.218 | 1.00 | 42.56 |
|    | ATOM | 5322 | O | HOH | W | 410 | 5.615   | 22.345 | 61.668 | 1.00 | 59.03 |
|    | ATOM | 5323 | O | HOH | W | 411 | -3.455  | 50.442 | 63.951 | 1.00 | 44.90 |
| 30 | ATOM | 5324 | O | HOH | W | 412 | 29.002  | 38.811 | 44.563 | 1.00 | 43.27 |
|    | ATOM | 5325 | O | HOH | W | 413 | 37.416  | 55.208 | 61.603 | 1.00 | 42.90 |
|    | ATOM | 5326 | O | HOH | W | 414 | 14.459  | 14.960 | 73.514 | 1.00 | 42.33 |
|    | ATOM | 5327 | O | HOH | W | 415 | 35.076  | 48.768 | 98.233 | 1.00 | 41.69 |
|    | ATOM | 5328 | O | HOH | W | 416 | 6.452   | 56.342 | 86.263 | 1.00 | 34.79 |
| 35 | ATOM | 5329 | O | HOH | W | 417 | 35.573  | 17.694 | 66.735 | 1.00 | 40.65 |
|    | ATOM | 5330 | O | HOH | W | 418 | 28.756  | 59.314 | 74.937 | 1.00 | 35.85 |
|    | ATOM | 5331 | O | HOH | W | 419 | 12.955  | 64.913 | 53.664 | 1.00 | 37.44 |
|    | ATOM | 5332 | O | HOH | W | 420 | 23.309  | 24.474 | 50.751 | 1.00 | 45.73 |
|    | ATOM | 5333 | O | HOH | W | 421 | 4.924   | 27.771 | 55.010 | 1.00 | 38.46 |
| 40 | ATOM | 5334 | O | HOH | W | 422 | 19.668  | 63.675 | 93.111 | 1.00 | 41.69 |
|    | ATOM | 5335 | O | HOH | W | 423 | 29.343  | 46.551 | 40.650 | 1.00 | 45.12 |
|    | ATOM | 5336 | O | HOH | W | 424 | 28.230  | 48.770 | 60.385 | 1.00 | 40.19 |
|    | ATOM | 5337 | O | HOH | W | 425 | 14.292  | 23.244 | 85.078 | 1.00 | 32.92 |
|    | ATOM | 5338 | O | HOH | W | 426 | 7.179   | 66.298 | 48.617 | 1.00 | 47.43 |
| 45 | ATOM | 5339 | O | HOH | W | 427 | -11.542 | 35.315 | 64.224 | 1.00 | 45.74 |
|    | ATOM | 5340 | O | HOH | W | 428 | -0.665  | 52.874 | 80.688 | 1.00 | 44.47 |
|    | ATOM | 5341 | O | HOH | W | 429 | -1.483  | 67.437 | 44.508 | 1.00 | 88.79 |
|    | ATOM | 5342 | O | HOH | W | 430 | 13.367  | 66.767 | 63.127 | 1.00 | 62.36 |
|    | ATOM | 5343 | O | HOH | W | 431 | 35.060  | 48.549 | 63.034 | 1.00 | 39.85 |
| 50 | ATOM | 5344 | O | HOH | W | 432 | 11.721  | 60.705 | 42.372 | 1.00 | 56.11 |
|    | ATOM | 5345 | O | HOH | W | 433 | 14.261  | 27.588 | 85.980 | 1.00 | 51.35 |
|    | ATOM | 5346 | O | HOH | W | 434 | 38.915  | 34.680 | 61.103 | 1.00 | 45.58 |
|    | ATOM | 5347 | O | HOH | W | 435 | 23.421  | 46.416 | 42.605 | 1.00 | 43.02 |
|    | ATOM | 5348 | O | HOH | W | 436 | 19.154  | 28.435 | 86.238 | 1.00 | 47.30 |
| 55 | ATOM | 5349 | O | HOH | W | 437 | 26.658  | 43.571 | 47.275 | 1.00 | 34.55 |
|    | ATOM | 5350 | O | HOH | W | 438 | 15.725  | 45.758 | 43.317 | 1.00 | 43.06 |
|    | ATOM | 5351 | O | HOH | W | 439 | 36.546  | 66.825 | 82.882 | 1.00 | 30.83 |
|    | ATOM | 5352 | O | HOH | W | 440 | 8.498   | 74.001 | 52.039 | 1.00 | 46.91 |
|    | ATOM | 5353 | O | HOH | W | 441 | 27.161  | 71.692 | 92.146 | 1.00 | 39.00 |
| 60 | ATOM | 5354 | O | HOH | W | 442 | 27.946  | 33.322 | 85.163 | 1.00 | 33.09 |
|    | ATOM | 5355 | O | HOH | W | 443 | 15.310  | 10.169 | 65.089 | 1.00 | 63.51 |
|    | ATOM | 5356 | O | HOH | W | 444 | -13.474 | 41.923 | 71.321 | 1.00 | 44.29 |
|    | ATOM | 5357 | O | HOH | W | 445 | -6.593  | 61.419 | 56.587 | 1.00 | 36.57 |
|    | ATOM | 5358 | O | HOH | W | 446 | -4.107  | 19.122 | 50.753 | 1.00 | 80.39 |
|    | ATOM | 5359 | O | HOH | W | 447 | 21.809  | 59.754 | 43.571 | 1.00 | 64.03 |
|    | ATOM | 5360 | O | HOH | W | 448 | 32.503  | 55.926 | 51.478 | 1.00 | 51.13 |
|    | ATOM | 5361 | O | HOH | W | 449 | 17.433  | 44.251 | 80.196 | 1.00 | 52.95 |
|    | ATOM | 5362 | O | HOH | W | 450 | -2.882  | 28.319 | 76.738 | 1.00 | 57.32 |



|    |      |      |   |           |         |        |         |      |       |
|----|------|------|---|-----------|---------|--------|---------|------|-------|
|    | ATOM | 5363 | O | HOH W 451 | 8.921   | 18.143 | 71.756  | 1.00 | 45.59 |
|    | ATOM | 5364 | O | HOH W 452 | 46.415  | 37.408 | 72.673  | 1.00 | 74.61 |
|    | ATOM | 5365 | O | HOH W 453 | 46.612  | 53.365 | 82.940  | 1.00 | 41.92 |
| 5  | ATOM | 5366 | O | HOH W 454 | 39.885  | 53.691 | 74.043  | 1.00 | 45.59 |
|    | ATOM | 5367 | O | HOH W 455 | 28.187  | 69.890 | 80.215  | 1.00 | 33.51 |
|    | ATOM | 5368 | O | HOH W 456 | 10.557  | 47.292 | 72.599  | 1.00 | 14.04 |
|    | ATOM | 5369 | O | HOH W 457 | -0.687  | 61.537 | 70.644  | 1.00 | 40.63 |
|    | ATOM | 5370 | O | HOH W 458 | 33.335  | 31.445 | 62.420  | 1.00 | 32.53 |
| 10 | ATOM | 5371 | O | HOH W 459 | 26.658  | 39.474 | 43.256  | 1.00 | 32.50 |
|    | ATOM | 5372 | O | HOH W 460 | 30.185  | 25.893 | 82.542  | 1.00 | 45.40 |
|    | ATOM | 5373 | O | HOH W 461 | 20.780  | 39.620 | 40.793  | 1.00 | 60.63 |
|    | ATOM | 5374 | O | HOH W 462 | -13.804 | 40.073 | 67.421  | 1.00 | 42.25 |
|    | ATOM | 5375 | O | HOH W 463 | 1.328   | 41.371 | 78.681  | 1.00 | 56.39 |
| 15 | ATOM | 5376 | O | HOH W 464 | 33.554  | 26.796 | 70.488  | 1.00 | 37.48 |
|    | ATOM | 5377 | O | HOH W 465 | 34.317  | 54.835 | 70.139  | 1.00 | 57.37 |
|    | ATOM | 5378 | O | HOH W 466 | 1.781   | 11.779 | 66.821  | 1.00 | 47.25 |
|    | ATOM | 5379 | O | HOH W 467 | 13.278  | 63.141 | 46.031  | 1.00 | 57.79 |
|    | ATOM | 5380 | O | HOH W 468 | 37.787  | 55.035 | 100.999 | 1.00 | 53.08 |
| 20 | ATOM | 5381 | O | HOH W 469 | 13.794  | 19.603 | 83.707  | 1.00 | 47.87 |
|    | ATOM | 5382 | O | HOH W 470 | 25.470  | 45.716 | 93.468  | 1.00 | 36.66 |
|    | ATOM | 5383 | O | HOH W 471 | 10.578  | 17.685 | 75.291  | 1.00 | 37.43 |
|    | ATOM | 5384 | O | HOH W 472 | 52.811  | 39.642 | 69.739  | 1.00 | 44.12 |
|    | ATOM | 5385 | O | HOH W 473 | 23.329  | 56.116 | 94.868  | 1.00 | 47.73 |
| 25 | ATOM | 5386 | O | HOH W 474 | 35.936  | 48.711 | 65.428  | 1.00 | 58.05 |
|    | ATOM | 5387 | O | HOH W 475 | 28.119  | 66.507 | 82.635  | 1.00 | 41.75 |
|    | ATOM | 5388 | O | HOH W 476 | -0.565  | 54.408 | 74.299  | 1.00 | 50.86 |
|    | ATOM | 5389 | O | HOH W 477 | 4.072   | 70.416 | 58.486  | 1.00 | 35.45 |
|    | ATOM | 5390 | O | HOH W 478 | -3.762  | 26.579 | 63.779  | 1.00 | 53.91 |
| 30 | ATOM | 5391 | O | HOH W 479 | 19.595  | 35.426 | 41.883  | 1.00 | 51.58 |
|    | ATOM | 5392 | O | HOH W 480 | 24.800  | 7.578  | 70.043  | 1.00 | 41.13 |
|    | ATOM | 5393 | O | HOH W 481 | 17.947  | 10.147 | 65.643  | 1.00 | 58.35 |
|    | ATOM | 5394 | O | HOH W 482 | 31.312  | 44.348 | 64.437  | 1.00 | 48.49 |
|    | ATOM | 5395 | O | HOH W 483 | 46.224  | 50.030 | 81.043  | 1.00 | 53.87 |
| 35 | ATOM | 5396 | O | HOH W 484 | 35.129  | 52.464 | 51.431  | 1.00 | 54.76 |
|    | ATOM | 5397 | O | HOH W 485 | 5.885   | 65.189 | 84.813  | 1.00 | 83.91 |
|    | ATOM | 5398 | O | HOH W 486 | 20.281  | 16.200 | 55.863  | 1.00 | 46.25 |
|    | ATOM | 5399 | O | HOH W 487 | -5.180  | 21.053 | 56.028  | 1.00 | 37.00 |
|    | ATOM | 5400 | O | HOH W 488 | -11.188 | 38.067 | 41.229  | 1.00 | 69.22 |
| 40 | ATOM | 5401 | O | HOH W 489 | 15.256  | 67.180 | 75.313  | 1.00 | 51.22 |
|    | ATOM | 5402 | O | HOH W 490 | 3.374   | 63.019 | 56.672  | 1.00 | 42.46 |
|    | ATOM | 5403 | O | HOH W 491 | 30.082  | 15.975 | 73.952  | 1.00 | 49.06 |
|    | ATOM | 5404 | O | HOH W 492 | -7.562  | 32.348 | 64.350  | 1.00 | 53.88 |
|    | ATOM | 5405 | O | HOH W 493 | 14.504  | 69.382 | 77.201  | 1.00 | 79.52 |
| 45 | ATOM | 5406 | O | HOH W 494 | 37.374  | 41.179 | 54.837  | 1.00 | 41.94 |
|    | ATOM | 5407 | O | HOH W 495 | 22.651  | 62.725 | 71.998  | 1.00 | 46.62 |
|    | ATOM | 5408 | O | HOH W 496 | 13.052  | 47.941 | 46.569  | 1.00 | 50.14 |
|    | ATOM | 5409 | O | HOH W 497 | -1.906  | 45.997 | 36.480  | 1.00 | 62.33 |
|    | ATOM | 5410 | O | HOH W 498 | 35.740  | 52.464 | 53.693  | 1.00 | 55.17 |
| 50 | ATOM | 5411 | O | HOH W 499 | 30.727  | 32.353 | 49.843  | 1.00 | 56.92 |
|    | ATOM | 5412 | O | HOH W 500 | 0.025   | 32.686 | 42.604  | 1.00 | 48.23 |
|    | ATOM | 5413 | O | HOH W 501 | 47.830  | 56.735 | 86.611  | 1.00 | 47.42 |
|    | ATOM | 5414 | O | HOH W 502 | 18.095  | 60.627 | 94.715  | 1.00 | 65.28 |
|    | ATOM | 5415 | O | HOH W 503 | 2.306   | 31.026 | 81.802  | 1.00 | 37.32 |
| 55 | ATOM | 5416 | O | HOH W 504 | -8.696  | 27.990 | 79.237  | 1.00 | 46.99 |
|    | ATOM | 5417 | O | HOH W 505 | 22.034  | 70.217 | 89.142  | 1.00 | 47.15 |
|    | ATOM | 5418 | O | HOH W 506 | 22.136  | 73.412 | 87.005  | 1.00 | 38.47 |
|    | ATOM | 5419 | O | HOH W 507 | -0.926  | 26.674 | 74.129  | 1.00 | 58.76 |
|    | ATOM | 5420 | O | HOH W 508 | -6.108  | 48.377 | 71.102  | 1.00 | 64.56 |
| 60 | ATOM | 5421 | O | HOH W 509 | 39.520  | 39.424 | 56.576  | 1.00 | 72.80 |
|    | ATOM | 5422 | O | HOH W 510 | -4.081  | 58.518 | 47.377  | 1.00 | 60.65 |
|    | ATOM | 5423 | O | HOH W 511 | 34.434  | 23.876 | 75.179  | 1.00 | 48.53 |
|    | ATOM | 5424 | O | HOH W 512 | 17.400  | 63.380 | 50.267  | 1.00 | 40.76 |
|    | ATOM | 5425 | O | HOH W 513 | 9.647   | 61.533 | 68.296  | 1.00 | 46.31 |
|    | ATOM | 5426 | O | HOH W 514 | 41.430  | 58.961 | 99.800  | 1.00 | 49.23 |



|    |      |      |   |           |         |        |        |      |        |
|----|------|------|---|-----------|---------|--------|--------|------|--------|
|    | ATOM | 5427 | O | HOH W 515 | 23.725  | 20.340 | 53.830 | 1.00 | 51.65  |
|    | ATOM | 5428 | O | HOH W 516 | 15.576  | 16.190 | 78.131 | 1.00 | 61.27  |
|    | ATOM | 5429 | O | HOH W 517 | 29.334  | 21.375 | 75.882 | 1.00 | 44.80  |
|    | ATOM | 5430 | O | HOH W 518 | -1.624  | 50.514 | 39.683 | 1.00 | 49.85  |
| 5  | ATOM | 5431 | O | HOH W 519 | 8.771   | 69.104 | 72.705 | 1.00 | 47.81  |
|    | ATOM | 5432 | O | HOH W 520 | -21.311 | 45.001 | 55.217 | 1.00 | 64.01  |
|    | ATOM | 5433 | O | HOH W 521 | -1.392  | 54.790 | 67.171 | 1.00 | 53.90  |
|    | ATOM | 5434 | O | HOH W 522 | 38.464  | 56.277 | 74.548 | 1.00 | 63.93  |
| 10 | ATOM | 5435 | O | HOH W 523 | 33.977  | 32.491 | 81.832 | 1.00 | 50.18  |
|    | ATOM | 5436 | O | HOH W 524 | 16.060  | 54.317 | 91.714 | 1.00 | 61.57  |
|    | ATOM | 5437 | O | HOH W 525 | 21.009  | 33.700 | 89.176 | 1.00 | 65.31  |
|    | ATOM | 5438 | O | HOH W 526 | 28.726  | 36.253 | 85.146 | 1.00 | 34.76  |
|    | ATOM | 5439 | O | HOH W 527 | 24.767  | 40.641 | 41.912 | 1.00 | 44.57  |
| 15 | ATOM | 5440 | O | HOH W 528 | 40.708  | 69.261 | 83.251 | 1.00 | 39.08  |
|    | ATOM | 5441 | O | HOH W 529 | 28.264  | 48.404 | 92.814 | 1.00 | 34.64  |
|    | ATOM | 5442 | O | HOH W 530 | 19.375  | 61.177 | 66.689 | 1.00 | 44.16  |
|    | ATOM | 5443 | O | HOH W 531 | 6.639   | 42.598 | 82.079 | 1.00 | 100.00 |
|    | ATOM | 5444 | O | HOH W 532 | 40.403  | 33.306 | 64.502 | 1.00 | 45.36  |
| 20 | ATOM | 5445 | O | HOH W 533 | 16.172  | 18.117 | 52.264 | 1.00 | 44.76  |
|    | ATOM | 5446 | O | HOH W 534 | 33.899  | 42.310 | 48.851 | 1.00 | 52.28  |
|    | ATOM | 5447 | O | HOH W 535 | 22.675  | 9.894  | 76.942 | 1.00 | 51.28  |
|    | ATOM | 5448 | O | HOH W 536 | -11.295 | 52.730 | 60.674 | 1.00 | 76.16  |
|    | ATOM | 5449 | O | HOH W 537 | 20.605  | 66.466 | 58.378 | 1.00 | 61.62  |
| 25 | ATOM | 5450 | O | HOH W 538 | 35.282  | 26.341 | 50.576 | 1.00 | 58.72  |
|    | ATOM | 5451 | O | HOH W 539 | -0.234  | 39.225 | 40.255 | 1.00 | 54.13  |
|    | ATOM | 5452 | O | HOH W 540 | 36.597  | 43.931 | 57.481 | 1.00 | 43.52  |
|    | ATOM | 5453 | O | HOH W 541 | 20.374  | 41.951 | 74.120 | 1.00 | 47.12  |
|    | ATOM | 5454 | O | HOH W 542 | 31.857  | 31.721 | 82.689 | 1.00 | 46.66  |
| 30 | ATOM | 5455 | O | HOH W 543 | 34.733  | 63.213 | 92.164 | 1.00 | 55.58  |
|    | ATOM | 5456 | O | HOH W 544 | -20.506 | 26.471 | 44.860 | 1.00 | 73.89  |
|    | ATOM | 5457 | O | HOH W 545 | 37.699  | 32.453 | 62.558 | 1.00 | 46.00  |
|    | ATOM | 5458 | O | HOH W 546 | 8.296   | 38.910 | 67.642 | 1.00 | 39.42  |
|    | ATOM | 5459 | O | HOH W 547 | 0.194   | 69.671 | 72.188 | 1.00 | 47.07  |
| 35 | ATOM | 5460 | O | HOH W 548 | 32.212  | 52.268 | 51.134 | 1.00 | 52.82  |
|    | ATOM | 5461 | O | HOH W 549 | 33.917  | 21.004 | 64.439 | 1.00 | 26.12  |
|    | ATOM | 5462 | O | HOH W 550 | 42.573  | 58.916 | 95.252 | 1.00 | 20.78  |
|    | ATOM | 5463 | O | HOH W 551 | 34.529  | 66.786 | 72.611 | 1.00 | 36.24  |

440225



Table 10: Structure coordinates of LTA<sub>4</sub> hydrolase-thiolamine complex

|    |        |         |         |           |       |        |         |                   |
|----|--------|---------|---------|-----------|-------|--------|---------|-------------------|
| 5  | CRYST  | 68.560  | 132.150 | 83.270    | 90.00 | 90.00  | 90.00   | P21212            |
|    | SCALE1 | 0.01459 | 0.00000 | 0.00000   |       |        | 0.00000 |                   |
|    | SCALE2 | 0.00000 | 0.00757 | 0.00000   |       |        | 0.00000 |                   |
|    | SCALE3 | 0.00000 | 0.00000 | 0.01201   |       |        | 0.00000 |                   |
|    |        |         |         |           |       |        |         |                   |
|    |        | Atom    | res.    | Chain No. | x     | y      | z       | occ B-factor      |
| 10 | ATOM   | 1       | N       | PRO A     | 1     | -0.593 | 16.387  | 63.494 1.00 97.99 |
|    | ATOM   | 2       | CA      | PRO A     | 1     | -1.890 | 16.918  | 63.874 1.00 97.22 |
|    | ATOM   | 3       | C       | PRO A     | 1     | -2.210 | 18.371  | 63.525 1.00100.00 |
|    | ATOM   | 4       | O       | PRO A     | 1     | -2.402 | 18.667  | 62.342 1.00100.00 |
| 15 | ATOM   | 5       | CB      | PRO A     | 1     | -2.130 | 16.551  | 65.332 1.00 97.81 |
|    | ATOM   | 6       | CG      | PRO A     | 1     | -1.221 | 15.355  | 65.583 1.00100.00 |
|    | ATOM   | 7       | CD      | PRO A     | 1     | -0.290 | 15.233  | 64.369 1.00 97.05 |
|    | ATOM   | 8       | N       | GLU A     | 2     | -2.216 | 19.272  | 64.556 1.00 96.95 |
| 20 | ATOM   | 9       | CA      | GLU A     | 2     | -2.569 | 20.678  | 64.314 1.00 95.71 |
|    | ATOM   | 10      | C       | GLU A     | 2     | -2.188 | 21.701  | 65.386 1.00 94.33 |
|    | ATOM   | 11      | O       | GLU A     | 2     | -2.512 | 21.542  | 66.562 1.00 93.21 |
|    | ATOM   | 12      | CB      | GLU A     | 2     | -4.105 | 20.768  | 64.214 1.00 97.26 |
| 25 | ATOM   | 13      | CG      | GLU A     | 2     | -4.587 | 21.732  | 63.125 1.00100.00 |
|    | ATOM   | 14      | CD      | GLU A     | 2     | -4.351 | 21.139  | 61.767 1.00100.00 |
|    | ATOM   | 15      | OE1     | GLU A     | 2     | -3.301 | 21.261  | 61.152 1.00100.00 |
|    | ATOM   | 16      | OE2     | GLU A     | 2     | -5.361 | 20.398  | 61.368 1.00100.00 |
| 30 | ATOM   | 17      | N       | ILE A     | 3     | -1.550 | 22.799  | 64.944 1.00 86.29 |
|    | ATOM   | 18      | CA      | ILE A     | 3     | -1.148 | 23.905  | 65.820 1.00 81.53 |
|    | ATOM   | 19      | C       | ILE A     | 3     | -2.006 | 25.154  | 65.661 1.00 75.68 |
|    | ATOM   | 20      | O       | ILE A     | 3     | -2.835 | 25.288  | 64.763 1.00 76.97 |
| 35 | ATOM   | 21      | CB      | ILE A     | 3     | 0.308  | 24.324  | 65.707 1.00 83.45 |
|    | ATOM   | 22      | CG1     | ILE A     | 3     | 0.452  | 25.521  | 64.759 1.00 83.63 |
|    | ATOM   | 23      | CG2     | ILE A     | 3     | 1.198  | 23.160  | 65.300 1.00 84.76 |
|    | ATOM   | 24      | CD1     | ILE A     | 3     | -0.184 | 25.361  | 63.375 1.00 91.36 |
| 40 | ATOM   | 25      | N       | VAL A     | 4     | -1.725 | 26.099  | 66.523 1.00 61.54 |
|    | ATOM   | 26      | CA      | VAL A     | 4     | -2.477 | 27.303  | 66.482 1.00 56.32 |
|    | ATOM   | 27      | C       | VAL A     | 4     | -1.658 | 28.552  | 66.623 1.00 50.98 |
|    | ATOM   | 28      | O       | VAL A     | 4     | -0.803 | 28.694  | 67.512 1.00 47.84 |
| 45 | ATOM   | 29      | CB      | VAL A     | 4     | -3.514 | 27.318  | 67.595 1.00 58.99 |
|    | ATOM   | 30      | CG1     | VAL A     | 4     | -3.735 | 28.754  | 68.047 1.00 58.40 |
|    | ATOM   | 31      | CG2     | VAL A     | 4     | -4.819 | 26.691  | 67.131 1.00 58.56 |
|    | ATOM   | 32      | N       | ASP A     | 5     | -2.012 | 29.486  | 65.732 1.00 39.38 |
| 50 | ATOM   | 33      | CA      | ASP A     | 5     | -1.403 | 30.782  | 65.763 1.00 32.64 |
|    | ATOM   | 34      | C       | ASP A     | 5     | -2.308 | 31.596  | 66.634 1.00 36.35 |
|    | ATOM   | 35      | O       | ASP A     | 5     | -3.343 | 32.051  | 66.171 1.00 38.30 |
|    | ATOM   | 36      | CB      | ASP A     | 5     | -1.252 | 31.492  | 64.400 1.00 30.79 |
| 55 | ATOM   | 37      | CG      | ASP A     | 5     | -0.251 | 32.581  | 64.563 1.00 29.96 |
|    | ATOM   | 38      | OD1     | ASP A     | 5     | -0.069 | 33.123  | 65.635 1.00 35.01 |
|    | ATOM   | 39      | OD2     | ASP A     | 5     | 0.457  | 32.831  | 63.493 1.00 29.81 |
|    | ATOM   | 40      | N       | THR A     | 6     | -1.931 | 31.745  | 67.903 1.00 32.32 |
| 60 | ATOM   | 41      | CA      | THR A     | 6     | -2.710 | 32.507  | 68.842 1.00 32.08 |
|    | ATOM   | 42      | C       | THR A     | 6     | -2.701 | 34.011  | 68.557 1.00 40.63 |
|    | ATOM   | 43      | O       | THR A     | 6     | -3.484 | 34.759  | 69.132 1.00 46.68 |
|    | ATOM   | 44      | CB      | THR A     | 6     | -2.357 | 32.171  | 70.295 1.00 44.71 |
| 65 | ATOM   | 45      | OG1     | THR A     | 6     | -0.967 | 32.322  | 70.505 1.00 51.05 |
|    | ATOM   | 46      | CG2     | THR A     | 6     | -2.789 | 30.741  | 70.604 1.00 35.79 |
|    | ATOM   | 47      | N       | CYS A     | 7     | -1.842 | 34.480  | 67.656 1.00 32.51 |
|    | ATOM   | 48      | CA      | CYS A     | 7     | -1.797 | 35.923  | 67.335 1.00 28.92 |
| 70 | ATOM   | 49      | C       | CYS A     | 7     | -2.627 | 36.329  | 66.129 1.00 31.49 |
|    | ATOM   | 50      | O       | CYS A     | 7     | -2.780 | 37.523  | 65.875 1.00 25.42 |
|    | ATOM   | 51      | CB      | CYS A     | 7     | -0.362 | 36.410  | 67.107 1.00 27.38 |
|    | ATOM   | 52      | SG      | CYS A     | 7     | 0.686  | 35.944  | 68.518 1.00 32.02 |
| 75 | ATOM   | 53      | N       | SER A     | 8     | -3.140 | 35.315  | 65.383 1.00 34.03 |
|    | ATOM   | 54      | CA      | SER A     | 8     | -3.940 | 35.508  | 64.158 1.00 32.97 |



|    |      |     |     |     |   |    |         |        |        |      |       |
|----|------|-----|-----|-----|---|----|---------|--------|--------|------|-------|
|    | ATOM | 55  | C   | SER | A | 8  | -5.410  | 35.136 | 64.264 | 1.00 | 33.52 |
|    | ATOM | 56  | O   | SER | A | 8  | -5.744  | 34.137 | 64.866 | 1.00 | 32.89 |
|    | ATOM | 57  | CB  | SER | A | 8  | -3.363  | 34.754 | 62.980 | 1.00 | 34.07 |
| 5  | ATOM | 58  | OG  | SER | A | 8  | -4.017  | 35.182 | 61.798 | 1.00 | 36.65 |
|    | ATOM | 59  | N   | LEU | A | 9  | -6.289  | 35.921 | 63.635 | 1.00 | 30.79 |
|    | ATOM | 60  | CA  | LEU | A | 9  | -7.724  | 35.649 | 63.672 | 1.00 | 31.91 |
|    | ATOM | 61  | C   | LEU | A | 9  | -8.198  | 35.009 | 62.377 | 1.00 | 36.07 |
|    | ATOM | 62  | O   | LEU | A | 9  | -9.359  | 34.626 | 62.216 | 1.00 | 38.61 |
| 10 | ATOM | 63  | CB  | LEU | A | 9  | -8.514  | 36.958 | 63.874 | 1.00 | 32.47 |
|    | ATOM | 64  | CG  | LEU | A | 9  | -8.306  | 37.688 | 65.212 | 1.00 | 35.39 |
|    | ATOM | 65  | CD1 | LEU | A | 9  | -9.113  | 38.983 | 65.193 | 1.00 | 32.27 |
|    | ATOM | 66  | CD2 | LEU | A | 9  | -8.746  | 36.816 | 66.397 | 1.00 | 33.25 |
|    | ATOM | 67  | N   | ALA | A | 10 | -7.273  | 34.933 | 61.443 | 1.00 | 28.63 |
| 15 | ATOM | 68  | CA  | ALA | A | 10 | -7.545  | 34.408 | 60.147 | 1.00 | 27.14 |
|    | ATOM | 69  | C   | ALA | A | 10 | -7.643  | 32.921 | 60.090 | 1.00 | 34.34 |
|    | ATOM | 70  | O   | ALA | A | 10 | -7.296  | 32.173 | 61.005 | 1.00 | 37.34 |
|    | ATOM | 71  | CB  | ALA | A | 10 | -6.551  | 34.936 | 59.100 | 1.00 | 27.72 |
|    | ATOM | 72  | N   | SER | A | 11 | -8.130  | 32.503 | 58.959 | 1.00 | 32.08 |
| 20 | ATOM | 73  | CA  | SER | A | 11 | -8.256  | 31.115 | 58.708 | 1.00 | 32.03 |
|    | ATOM | 74  | C   | SER | A | 11 | -6.838  | 30.519 | 58.656 | 1.00 | 32.67 |
|    | ATOM | 75  | O   | SER | A | 11 | -5.927  | 31.028 | 57.986 | 1.00 | 29.29 |
|    | ATOM | 76  | CB  | SER | A | 11 | -9.013  | 30.934 | 57.401 | 1.00 | 38.42 |
|    | ATOM | 77  | OG  | SER | A | 11 | -10.391 | 30.728 | 57.648 | 1.00 | 44.17 |
| 25 | ATOM | 78  | N   | PRO | A | 12 | -6.651  | 29.440 | 59.387 | 1.00 | 29.14 |
|    | ATOM | 79  | CA  | PRO | A | 12 | -5.370  | 28.786 | 59.476 | 1.00 | 26.83 |
|    | ATOM | 80  | C   | PRO | A | 12 | -4.935  | 28.176 | 58.173 | 1.00 | 32.64 |
|    | ATOM | 81  | O   | PRO | A | 12 | -5.737  | 28.007 | 57.284 | 1.00 | 35.89 |
|    | ATOM | 82  | CB  | PRO | A | 12 | -5.544  | 27.698 | 60.540 | 1.00 | 28.28 |
| 30 | ATOM | 83  | CG  | PRO | A | 12 | -7.029  | 27.571 | 60.843 | 1.00 | 32.92 |
|    | ATOM | 84  | CD  | PRO | A | 12 | -7.731  | 28.587 | 59.952 | 1.00 | 30.42 |
|    | ATOM | 85  | N   | ALA | A | 13 | -3.645  | 27.836 | 58.063 | 1.00 | 30.63 |
|    | ATOM | 86  | CA  | ALA | A | 13 | -3.066  | 27.236 | 56.855 | 1.00 | 28.36 |
|    | ATOM | 87  | C   | ALA | A | 13 | -3.644  | 25.852 | 56.576 | 1.00 | 33.99 |
| 35 | ATOM | 88  | O   | ALA | A | 13 | -3.455  | 25.240 | 55.528 | 1.00 | 31.60 |
|    | ATOM | 89  | CB  | ALA | A | 13 | -1.561  | 27.133 | 57.050 | 1.00 | 27.68 |
|    | ATOM | 90  | N   | SER | A | 14 | -4.338  | 25.352 | 57.571 | 1.00 | 31.10 |
|    | ATOM | 91  | CA  | SER | A | 14 | -4.919  | 24.069 | 57.469 | 1.00 | 30.66 |
|    | ATOM | 92  | C   | SER | A | 14 | -6.242  | 24.133 | 56.753 | 1.00 | 37.86 |
| 40 | ATOM | 93  | O   | SER | A | 14 | -6.768  | 23.118 | 56.328 | 1.00 | 45.79 |
|    | ATOM | 94  | CB  | SER | A | 14 | -5.005  | 23.386 | 58.825 | 1.00 | 34.33 |
|    | ATOM | 95  | OG  | SER | A | 14 | -6.006  | 23.978 | 59.621 | 1.00 | 41.01 |
|    | ATOM | 96  | N   | VAL | A | 15 | -6.785  | 25.327 | 56.630 | 1.00 | 32.80 |
|    | ATOM | 97  | CA  | VAL | A | 15 | -8.036  | 25.529 | 55.917 | 1.00 | 31.81 |
| 45 | ATOM | 98  | C   | VAL | A | 15 | -7.777  | 26.107 | 54.507 | 1.00 | 34.70 |
|    | ATOM | 99  | O   | VAL | A | 15 | -8.241  | 25.576 | 53.494 | 1.00 | 31.96 |
|    | ATOM | 100 | CB  | VAL | A | 15 | -9.033  | 26.336 | 56.720 | 1.00 | 33.07 |
|    | ATOM | 101 | CG1 | VAL | A | 15 | -10.272 | 26.638 | 55.861 | 1.00 | 33.31 |
|    | ATOM | 102 | CG2 | VAL | A | 15 | -9.412  | 25.538 | 57.949 | 1.00 | 30.32 |
| 50 | ATOM | 103 | N   | CYS | A | 16 | -6.990  | 27.183 | 54.453 | 1.00 | 33.85 |
|    | ATOM | 104 | CA  | CYS | A | 16 | -6.602  | 27.826 | 53.189 | 1.00 | 38.27 |
|    | ATOM | 105 | C   | CYS | A | 16 | -5.206  | 28.388 | 53.265 | 1.00 | 37.14 |
|    | ATOM | 106 | O   | CYS | A | 16 | -4.616  | 28.534 | 54.322 | 1.00 | 39.70 |
|    | ATOM | 107 | CB  | CYS | A | 16 | -7.589  | 28.870 | 52.581 | 1.00 | 42.09 |
| 55 | ATOM | 108 | SG  | CYS | A | 16 | -7.844  | 30.418 | 53.540 | 1.00 | 47.38 |
|    | ATOM | 109 | N   | ARG | A | 17 | -4.679  | 28.722 | 52.132 | 1.00 | 32.10 |
|    | ATOM | 110 | CA  | ARG | A | 17 | -3.349  | 29.262 | 52.101 | 1.00 | 32.54 |
|    | ATOM | 111 | C   | ARG | A | 17 | -3.210  | 30.307 | 51.005 | 1.00 | 34.56 |
|    | ATOM | 112 | O   | ARG | A | 17 | -3.511  | 30.065 | 49.842 | 1.00 | 35.07 |
| 60 | ATOM | 113 | CB  | ARG | A | 17 | -2.371  | 28.152 | 51.758 | 1.00 | 36.83 |
|    | ATOM | 114 | CG  | ARG | A | 17 | -1.779  | 27.391 | 52.915 | 1.00 | 40.61 |
|    | ATOM | 115 | CD  | ARG | A | 17 | -1.472  | 25.970 | 52.503 | 1.00 | 27.18 |
|    | ATOM | 116 | NE  | ARG | A | 17 | -1.963  | 25.026 | 53.501 | 1.00 | 52.41 |
|    | ATOM | 117 | CZ  | ARG | A | 17 | -1.244  | 24.036 | 54.035 | 1.00 | 69.41 |
|    | ATOM | 118 | NH1 | ARG | A | 17 | 0.020   | 23.812 | 53.683 | 1.00 | 54.86 |



|    |      |     |     |     |   |    |        |        |        |      |        |
|----|------|-----|-----|-----|---|----|--------|--------|--------|------|--------|
|    | ATOM | 119 | NH2 | ARG | A | 17 | -1.810 | 23.246 | 54.952 | 1.00 | 49.68  |
|    | ATOM | 120 | N   | THR | A | 18 | -2.711 | 31.454 | 51.378 | 1.00 | 27.06  |
|    | ATOM | 121 | CA  | THR | A | 18 | -2.489 | 32.477 | 50.428 | 1.00 | 26.12  |
| 5  | ATOM | 122 | C   | THR | A | 18 | -1.250 | 32.110 | 49.653 | 1.00 | 30.83  |
|    | ATOM | 123 | O   | THR | A | 18 | -0.174 | 31.964 | 50.194 | 1.00 | 29.06  |
|    | ATOM | 124 | CB  | THR | A | 18 | -2.276 | 33.810 | 51.134 | 1.00 | 34.27  |
|    | ATOM | 125 | OG1 | THR | A | 18 | -3.481 | 34.261 | 51.738 | 1.00 | 32.95  |
|    | ATOM | 126 | CG2 | THR | A | 18 | -1.730 | 34.839 | 50.156 | 1.00 | 35.91  |
| 10 | ATOM | 127 | N   | LYS | A | 19 | -1.408 | 31.955 | 48.365 | 1.00 | 31.55  |
|    | ATOM | 128 | CA  | LYS | A | 19 | -0.298 | 31.615 | 47.511 | 1.00 | 31.74  |
|    | ATOM | 129 | C   | LYS | A | 19 | 0.359  | 32.848 | 46.906 | 1.00 | 33.90  |
|    | ATOM | 130 | O   | LYS | A | 19 | 1.513  | 32.834 | 46.520 | 1.00 | 34.57  |
|    | ATOM | 131 | CB  | LYS | A | 19 | -0.795 | 30.697 | 46.398 | 1.00 | 36.08  |
| 15 | ATOM | 132 | CG  | LYS | A | 19 | -1.332 | 29.368 | 46.924 | 1.00 | 62.54  |
|    | ATOM | 133 | CD  | LYS | A | 19 | -0.281 | 28.257 | 47.057 | 1.00 | 82.23  |
|    | ATOM | 134 | CE  | LYS | A | 19 | 0.093  | 27.880 | 48.496 | 1.00 | 77.50  |
|    | ATOM | 135 | NZ  | LYS | A | 19 | 1.553  | 27.849 | 48.745 | 1.00 | 55.63  |
|    | ATOM | 136 | N   | HIS | A | 20 | -0.387 | 33.928 | 46.810 | 1.00 | 31.40  |
| 20 | ATOM | 137 | CA  | HIS | A | 20 | 0.160  | 35.122 | 46.198 | 1.00 | 29.22  |
|    | ATOM | 138 | C   | HIS | A | 20 | -0.655 | 36.345 | 46.517 | 1.00 | 34.68  |
|    | ATOM | 139 | O   | HIS | A | 20 | -1.833 | 36.239 | 46.846 | 1.00 | 35.34  |
|    | ATOM | 140 | CB  | HIS | A | 20 | 0.123  | 34.956 | 44.666 | 1.00 | 26.47  |
|    | ATOM | 141 | CG  | HIS | A | 20 | 0.865  | 36.022 | 43.970 | 1.00 | 26.77  |
| 25 | ATOM | 142 | ND1 | HIS | A | 20 | 2.249  | 36.046 | 43.980 | 1.00 | 28.92  |
|    | ATOM | 143 | CD2 | HIS | A | 20 | 0.415  | 37.091 | 43.280 | 1.00 | 27.43  |
|    | ATOM | 144 | CE1 | HIS | A | 20 | 2.622  | 37.126 | 43.301 | 1.00 | 28.21  |
|    | ATOM | 145 | NE2 | HIS | A | 20 | 1.536  | 37.781 | 42.865 | 1.00 | 28.18  |
|    | ATOM | 146 | N   | LEU | A | 21 | 0.000  | 37.492 | 46.390 | 1.00 | 30.14  |
| 30 | ATOM | 147 | CA  | LEU | A | 21 | -0.596 | 38.782 | 46.610 | 1.00 | 31.02  |
|    | ATOM | 148 | C   | LEU | A | 21 | -0.134 | 39.786 | 45.562 | 1.00 | 38.34  |
|    | ATOM | 149 | O   | LEU | A | 21 | 1.073  | 39.952 | 45.312 | 1.00 | 37.30  |
|    | ATOM | 150 | CB  | LEU | A | 21 | -0.342 | 39.363 | 47.999 | 1.00 | 31.30  |
|    | ATOM | 151 | CG  | LEU | A | 21 | -0.611 | 40.880 | 48.047 | 1.00 | 32.33  |
| 35 | ATOM | 152 | CD1 | LEU | A | 21 | -2.088 | 41.192 | 48.324 | 1.00 | 27.10  |
|    | ATOM | 153 | CD2 | LEU | A | 21 | 0.277  | 41.522 | 49.100 | 1.00 | 32.86  |
|    | ATOM | 154 | N   | HIS | A | 22 | -1.127 | 40.442 | 44.951 | 1.00 | 35.47  |
|    | ATOM | 155 | CA  | HIS | A | 22 | -0.895 | 41.452 | 43.920 | 1.00 | 34.24  |
|    | ATOM | 156 | C   | HIS | A | 22 | -1.249 | 42.742 | 44.550 | 1.00 | 33.99  |
| 40 | ATOM | 157 | O   | HIS | A | 22 | -2.402 | 42.957 | 44.905 | 1.00 | 35.72  |
|    | ATOM | 158 | CB  | HIS | A | 22 | -1.720 | 41.244 | 42.624 | 1.00 | 33.38  |
|    | ATOM | 159 | CG  | HIS | A | 22 | -1.350 | 42.256 | 41.615 | 1.00 | 35.97  |
|    | ATOM | 160 | ND1 | HIS | A | 22 | -0.030 | 42.576 | 41.384 | 1.00 | 38.81  |
|    | ATOM | 161 | CD2 | HIS | A | 22 | -2.125 | 43.043 | 40.830 | 1.00 | 39.07  |
| 45 | ATOM | 162 | CE1 | HIS | A | 22 | -0.019 | 43.534 | 40.462 | 1.00 | 38.66  |
|    | ATOM | 163 | NE2 | HIS | A | 22 | -1.262 | 43.829 | 40.103 | 1.00 | 39.13  |
|    | ATOM | 164 | N   | LEU | A | 23 | -0.235 | 43.539 | 44.757 | 1.00 | 30.17  |
|    | ATOM | 165 | CA  | LEU | A | 23 | -0.416 | 44.793 | 45.405 | 1.00 | 33.32  |
|    | ATOM | 166 | C   | LEU | A | 23 | -0.203 | 45.949 | 44.440 | 1.00 | 44.46  |
| 50 | ATOM | 167 | O   | LEU | A | 23 | 0.828  | 46.068 | 43.761 | 1.00 | 44.06  |
|    | ATOM | 168 | CB  | LEU | A | 23 | 0.446  | 44.882 | 46.680 | 1.00 | 33.72  |
|    | ATOM | 169 | CG  | LEU | A | 23 | -0.141 | 45.682 | 47.871 | 1.00 | 33.15  |
|    | ATOM | 170 | CD1 | LEU | A | 23 | 0.780  | 46.835 | 48.172 | 1.00 | 26.07  |
|    | ATOM | 171 | CD2 | LEU | A | 23 | -1.539 | 46.213 | 47.609 | 1.00 | 35.39  |
| 55 | ATOM | 172 | N   | ARG | A | 24 | -1.256 | 46.765 | 44.395 | 1.00 | 42.83  |
|    | ATOM | 173 | CA  | ARG | A | 24 | -1.406 | 47.964 | 43.596 | 1.00 | 41.79  |
|    | ATOM | 174 | C   | ARG | A | 24 | -1.930 | 49.005 | 44.562 | 1.00 | 39.15  |
|    | ATOM | 175 | O   | ARG | A | 24 | -3.025 | 48.859 | 45.107 | 1.00 | 39.85  |
|    | ATOM | 176 | CB  | ARG | A | 24 | -2.458 | 47.716 | 42.504 | 1.00 | 46.35  |
| 60 | ATOM | 177 | CG  | ARG | A | 24 | -2.054 | 46.750 | 41.382 | 1.00 | 50.50  |
|    | ATOM | 178 | CD  | ARG | A | 24 | -2.754 | 47.058 | 40.043 | 1.00 | 80.27  |
|    | ATOM | 179 | NE  | ARG | A | 24 | -4.200 | 46.798 | 40.062 | 1.00 | 95.12  |
|    | ATOM | 180 | CZ  | ARG | A | 24 | -5.152 | 47.703 | 39.826 | 1.00 | 100.00 |
|    | ATOM | 181 | NH1 | ARG | A | 24 | -4.863 | 48.973 | 39.483 | 1.00 | 100.00 |
|    | ATOM | 182 | NH2 | ARG | A | 24 | -6.432 | 47.326 | 39.865 | 1.00 | 100.00 |



|    |      |     |     |     |   |    |        |        |        |      |        |
|----|------|-----|-----|-----|---|----|--------|--------|--------|------|--------|
|    | ATOM | 183 | N   | CYS | A | 25 | -1.164 | 50.028 | 44.844 | 1.00 | 32.39  |
|    | ATOM | 184 | CA  | CYS | A | 25 | -1.698 | 50.969 | 45.813 | 1.00 | 33.30  |
|    | ATOM | 185 | C   | CYS | A | 25 | -1.061 | 52.325 | 45.724 | 1.00 | 34.82  |
| 5  | ATOM | 186 | O   | CYS | A | 25 | -0.012 | 52.514 | 45.076 | 1.00 | 31.03  |
|    | ATOM | 187 | CB  | CYS | A | 25 | -1.503 | 50.440 | 47.257 | 1.00 | 34.67  |
|    | ATOM | 188 | SG  | CYS | A | 25 | 0.231  | 50.529 | 47.798 | 1.00 | 38.07  |
|    | ATOM | 189 | N   | SER | A | 26 | -1.711 | 53.257 | 46.418 | 1.00 | 34.39  |
|    | ATOM | 190 | CA  | SER | A | 26 | -1.196 | 54.601 | 46.437 | 1.00 | 36.77  |
| 10 | ATOM | 191 | C   | SER | A | 26 | -0.963 | 55.133 | 47.821 | 1.00 | 39.85  |
|    | ATOM | 192 | O   | SER | A | 26 | -1.738 | 54.853 | 48.757 | 1.00 | 37.56  |
|    | ATOM | 193 | CB  | SER | A | 26 | -1.889 | 55.600 | 45.530 | 1.00 | 42.70  |
|    | ATOM | 194 | OG  | SER | A | 26 | -0.899 | 56.330 | 44.824 | 1.00 | 61.74  |
|    | ATOM | 195 | N   | VAL | A | 27 | 0.133  | 55.897 | 47.886 | 1.00 | 39.43  |
| 15 | ATOM | 196 | CA  | VAL | A | 27 | 0.624  | 56.583 | 49.081 | 1.00 | 41.31  |
|    | ATOM | 197 | C   | VAL | A | 27 | 0.209  | 58.043 | 49.082 | 1.00 | 44.32  |
|    | ATOM | 198 | O   | VAL | A | 27 | 0.562  | 58.799 | 48.187 | 1.00 | 45.24  |
|    | ATOM | 199 | CB  | VAL | A | 27 | 2.135  | 56.531 | 49.207 | 1.00 | 46.35  |
|    | ATOM | 200 | CG1 | VAL | A | 27 | 2.524  | 57.207 | 50.522 | 1.00 | 45.62  |
|    | ATOM | 201 | CG2 | VAL | A | 27 | 2.592  | 55.079 | 49.178 | 1.00 | 47.20  |
| 20 | ATOM | 202 | N   | ASP | A | 28 | -0.553 | 58.417 | 50.093 | 1.00 | 37.94  |
|    | ATOM | 203 | CA  | ASP | A | 28 | -1.040 | 59.764 | 50.237 | 1.00 | 35.28  |
|    | ATOM | 204 | C   | ASP | A | 28 | -0.595 | 60.366 | 51.538 | 1.00 | 33.85  |
|    | ATOM | 205 | O   | ASP | A | 28 | -1.181 | 60.099 | 52.598 | 1.00 | 28.52  |
| 25 | ATOM | 206 | CB  | ASP | A | 28 | -2.559 | 59.807 | 50.189 | 1.00 | 37.09  |
|    | ATOM | 207 | CG  | ASP | A | 28 | -3.055 | 61.205 | 50.095 | 1.00 | 55.20  |
|    | ATOM | 208 | OD1 | ASP | A | 28 | -2.611 | 62.119 | 50.767 | 1.00 | 59.17  |
|    | ATOM | 209 | OD2 | ASP | A | 28 | -3.993 | 61.335 | 49.192 | 1.00 | 61.41  |
|    | ATOM | 210 | N   | PHE | A | 29 | 0.436  | 61.174 | 51.405 | 1.00 | 36.42  |
| 30 | ATOM | 211 | CA  | PHE | A | 29 | 1.044  | 61.888 | 52.512 | 1.00 | 43.07  |
|    | ATOM | 212 | C   | PHE | A | 29 | 0.105  | 62.928 | 53.077 | 1.00 | 51.14  |
|    | ATOM | 213 | O   | PHE | A | 29 | 0.161  | 63.279 | 54.257 | 1.00 | 51.35  |
|    | ATOM | 214 | CB  | PHE | A | 29 | 2.410  | 62.517 | 52.143 | 1.00 | 47.77  |
|    | ATOM | 215 | CG  | PHE | A | 29 | 3.519  | 61.485 | 52.079 | 1.00 | 50.86  |
| 35 | ATOM | 216 | CD1 | PHE | A | 29 | 4.066  | 60.957 | 53.247 | 1.00 | 52.08  |
|    | ATOM | 217 | CD2 | PHE | A | 29 | 3.996  | 61.001 | 50.863 | 1.00 | 53.94  |
|    | ATOM | 218 | CE1 | PHE | A | 29 | 5.075  | 59.995 | 53.215 | 1.00 | 52.83  |
|    | ATOM | 219 | CE2 | PHE | A | 29 | 5.013  | 60.046 | 50.813 | 1.00 | 56.46  |
|    | ATOM | 220 | CZ  | PHE | A | 29 | 5.559  | 59.538 | 51.992 | 1.00 | 53.39  |
| 40 | ATOM | 221 | N   | THR | A | 30 | -0.766 | 63.420 | 52.220 | 1.00 | 47.10  |
|    | ATOM | 222 | CA  | THR | A | 30 | -1.718 | 64.386 | 52.654 | 1.00 | 45.48  |
|    | ATOM | 223 | C   | THR | A | 30 | -2.788 | 63.715 | 53.509 | 1.00 | 48.41  |
|    | ATOM | 224 | O   | THR | A | 30 | -3.045 | 64.082 | 54.649 | 1.00 | 48.64  |
|    | ATOM | 225 | CB  | THR | A | 30 | -2.283 | 65.097 | 51.434 | 1.00 | 54.06  |
| 45 | ATOM | 226 | OG1 | THR | A | 30 | -1.428 | 66.186 | 51.107 | 1.00 | 50.68  |
|    | ATOM | 227 | CG2 | THR | A | 30 | -3.697 | 65.568 | 51.745 | 1.00 | 60.28  |
|    | ATOM | 228 | N   | ARG | A | 31 | -3.392 | 62.683 | 52.978 | 1.00 | 46.66  |
|    | ATOM | 229 | CA  | ARG | A | 31 | -4.404 | 61.987 | 53.734 | 1.00 | 47.88  |
|    | ATOM | 230 | C   | ARG | A | 31 | -3.826 | 60.999 | 54.750 | 1.00 | 45.46  |
| 50 | ATOM | 231 | O   | ARG | A | 31 | -4.590 | 60.468 | 55.551 | 1.00 | 41.52  |
|    | ATOM | 232 | CB  | ARG | A | 31 | -5.335 | 61.214 | 52.805 | 1.00 | 56.73  |
|    | ATOM | 233 | CG  | ARG | A | 31 | -5.950 | 62.065 | 51.700 | 1.00 | 84.16  |
|    | ATOM | 234 | CD  | ARG | A | 31 | -7.338 | 61.568 | 51.284 | 1.00 | 100.00 |
|    | ATOM | 235 | NE  | ARG | A | 31 | -7.344 | 60.450 | 50.327 | 1.00 | 100.00 |
| 55 | ATOM | 236 | CZ  | ARG | A | 31 | -8.148 | 60.371 | 49.251 | 1.00 | 100.00 |
|    | ATOM | 237 | NH1 | ARG | A | 31 | -9.034 | 61.324 | 48.944 | 1.00 | 100.00 |
|    | ATOM | 238 | NH2 | ARG | A | 31 | -8.062 | 59.298 | 48.460 | 1.00 | 100.00 |
|    | ATOM | 239 | N   | ARG | A | 32 | -2.489 | 60.752 | 54.683 | 1.00 | 39.71  |
|    | ATOM | 240 | CA  | ARG | A | 32 | -1.751 | 59.798 | 55.531 | 1.00 | 39.09  |
| 60 | ATOM | 241 | C   | ARG | A | 32 | -2.324 | 58.411 | 55.379 | 1.00 | 39.62  |
|    | ATOM | 242 | O   | ARG | A | 32 | -2.495 | 57.655 | 56.337 | 1.00 | 33.10  |
|    | ATOM | 243 | CB  | ARG | A | 32 | -1.523 | 60.115 | 57.022 | 1.00 | 37.14  |
|    | ATOM | 244 | CG  | ARG | A | 32 | -1.197 | 61.569 | 57.337 | 1.00 | 71.25  |
|    | ATOM | 245 | CD  | ARG | A | 32 | 0.277  | 61.834 | 57.686 | 1.00 | 100.00 |
|    | ATOM | 246 | NE  | ARG | A | 32 | 0.703  | 61.299 | 58.986 | 1.00 | 100.00 |



|    |      |     |     |     |   |    |        |        |        |      |       |
|----|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|
|    | ATOM | 247 | CZ  | ARG | A | 32 | 1.284  | 62.005 | 59.961 | 1.00 | 79.51 |
|    | ATOM | 248 | NH1 | ARG | A | 32 | 1.522  | 63.308 | 59.831 | 1.00 | 55.73 |
|    | ATOM | 249 | NH2 | ARG | A | 32 | 1.626  | 61.387 | 61.098 | 1.00 | 44.96 |
| 5  | ATOM | 250 | N   | THR | A | 33 | -2.612 | 58.068 | 54.139 | 1.00 | 39.83 |
|    | ATOM | 251 | CA  | THR | A | 33 | -3.162 | 56.752 | 53.902 | 1.00 | 39.31 |
|    | ATOM | 252 | C   | THR | A | 33 | -2.543 | 56.010 | 52.760 | 1.00 | 41.13 |
|    | ATOM | 253 | O   | THR | A | 33 | -1.853 | 56.574 | 51.926 | 1.00 | 42.93 |
|    | ATOM | 254 | CB  | THR | A | 33 | -4.635 | 56.835 | 53.641 | 1.00 | 43.44 |
| 10 | ATOM | 255 | OG1 | THR | A | 33 | -4.798 | 57.636 | 52.468 | 1.00 | 40.17 |
|    | ATOM | 256 | CG2 | THR | A | 33 | -5.245 | 57.468 | 54.880 | 1.00 | 38.71 |
|    | ATOM | 257 | N   | LEU | A | 34 | -2.822 | 54.717 | 52.762 | 1.00 | 35.26 |
|    | ATOM | 258 | CA  | LEU | A | 34 | -2.372 | 53.799 | 51.745 | 1.00 | 35.20 |
|    | ATOM | 259 | C   | LEU | A | 34 | -3.632 | 53.293 | 51.098 | 1.00 | 32.49 |
| 15 | ATOM | 260 | O   | LEU | A | 34 | -4.474 | 52.670 | 51.751 | 1.00 | 30.96 |
|    | ATOM | 261 | CB  | LEU | A | 34 | -1.522 | 52.651 | 52.322 | 1.00 | 37.07 |
|    | ATOM | 262 | CG  | LEU | A | 34 | -0.149 | 52.571 | 51.685 | 1.00 | 42.99 |
|    | ATOM | 263 | CD1 | LEU | A | 34 | 0.648  | 51.425 | 52.285 | 1.00 | 40.58 |
|    | ATOM | 264 | CD2 | LEU | A | 34 | -0.360 | 52.302 | 50.208 | 1.00 | 50.83 |
| 20 | ATOM | 265 | N   | THR | A | 35 | -3.800 | 53.632 | 49.838 | 1.00 | 28.72 |
|    | ATOM | 266 | CA  | THR | A | 35 | -5.017 | 53.228 | 49.198 | 1.00 | 31.26 |
|    | ATOM | 267 | C   | THR | A | 35 | -4.838 | 52.329 | 48.013 | 1.00 | 36.54 |
|    | ATOM | 268 | O   | THR | A | 35 | -3.940 | 52.546 | 47.187 | 1.00 | 34.70 |
|    | ATOM | 269 | CB  | THR | A | 35 | -5.877 | 54.427 | 48.813 | 1.00 | 44.88 |
| 25 | ATOM | 270 | OG1 | THR | A | 35 | -5.484 | 55.549 | 49.579 | 1.00 | 58.59 |
|    | ATOM | 271 | CG2 | THR | A | 35 | -7.324 | 54.094 | 49.109 | 1.00 | 49.42 |
|    | ATOM | 272 | N   | GLY | A | 36 | -5.726 | 51.329 | 47.950 | 1.00 | 32.57 |
|    | ATOM | 273 | CA  | GLY | A | 36 | -5.696 | 50.405 | 46.837 | 1.00 | 33.89 |
|    | ATOM | 274 | C   | GLY | A | 36 | -6.418 | 49.074 | 46.993 | 1.00 | 34.50 |
| 30 | ATOM | 275 | O   | GLY | A | 36 | -7.441 | 48.919 | 47.678 | 1.00 | 31.78 |
|    | ATOM | 276 | N   | THR | A | 37 | -5.836 | 48.103 | 46.293 | 1.00 | 35.93 |
|    | ATOM | 277 | CA  | THR | A | 37 | -6.327 | 46.723 | 46.281 | 1.00 | 36.12 |
|    | ATOM | 278 | C   | THR | A | 37 | -5.268 | 45.696 | 46.473 | 1.00 | 35.67 |
|    | ATOM | 279 | O   | THR | A | 37 | -4.155 | 45.795 | 45.964 | 1.00 | 33.86 |
| 35 | ATOM | 280 | CB  | THR | A | 37 | -7.119 | 46.306 | 45.050 | 1.00 | 42.21 |
|    | ATOM | 281 | OG1 | THR | A | 37 | -6.507 | 46.804 | 43.870 | 1.00 | 30.98 |
|    | ATOM | 282 | CG2 | THR | A | 37 | -8.547 | 46.793 | 45.229 | 1.00 | 50.03 |
|    | ATOM | 283 | N   | ALA | A | 38 | -5.687 | 44.705 | 47.220 | 1.00 | 32.95 |
|    | ATOM | 284 | CA  | ALA | A | 38 | -4.886 | 43.570 | 47.533 | 1.00 | 33.45 |
| 40 | ATOM | 285 | C   | ALA | A | 38 | -5.481 | 42.374 | 46.824 | 1.00 | 35.47 |
|    | ATOM | 286 | O   | ALA | A | 38 | -6.580 | 41.906 | 47.151 | 1.00 | 32.91 |
|    | ATOM | 287 | CB  | ALA | A | 38 | -4.845 | 43.341 | 49.044 | 1.00 | 33.72 |
|    | ATOM | 288 | N   | ALA | A | 39 | -4.764 | 41.874 | 45.834 | 1.00 | 32.70 |
|    | ATOM | 289 | CA  | ALA | A | 39 | -5.274 | 40.702 | 45.140 | 1.00 | 31.59 |
| 45 | ATOM | 290 | C   | ALA | A | 39 | -4.692 | 39.464 | 45.770 | 1.00 | 32.11 |
|    | ATOM | 291 | O   | ALA | A | 39 | -3.514 | 39.147 | 45.608 | 1.00 | 32.46 |
|    | ATOM | 292 | CB  | ALA | A | 39 | -4.934 | 40.729 | 43.662 | 1.00 | 32.13 |
|    | ATOM | 293 | N   | LEU | A | 40 | -5.505 | 38.774 | 46.508 | 1.00 | 27.06 |
|    | ATOM | 294 | CA  | LEU | A | 40 | -5.001 | 37.593 | 47.155 | 1.00 | 29.04 |
| 50 | ATOM | 295 | C   | LEU | A | 40 | -5.331 | 36.322 | 46.364 | 1.00 | 36.88 |
|    | ATOM | 296 | O   | LEU | A | 40 | -6.485 | 36.100 | 45.963 | 1.00 | 28.89 |
|    | ATOM | 297 | CB  | LEU | A | 40 | -5.587 | 37.451 | 48.600 | 1.00 | 29.39 |
|    | ATOM | 298 | CG  | LEU | A | 40 | -5.303 | 38.598 | 49.559 | 1.00 | 31.39 |
|    | ATOM | 299 | CD1 | LEU | A | 40 | -5.435 | 38.063 | 50.970 | 1.00 | 32.62 |
| 55 | ATOM | 300 | CD2 | LEU | A | 40 | -3.879 | 39.019 | 49.355 | 1.00 | 31.60 |
|    | ATOM | 301 | N   | THR | A | 41 | -4.310 | 35.470 | 46.165 | 1.00 | 42.40 |
|    | ATOM | 302 | CA  | THR | A | 41 | -4.523 | 34.210 | 45.488 | 1.00 | 43.93 |
|    | ATOM | 303 | C   | THR | A | 41 | -4.548 | 33.155 | 46.552 | 1.00 | 43.75 |
|    | ATOM | 304 | O   | THR | A | 41 | -3.510 | 32.827 | 47.115 | 1.00 | 45.22 |
| 60 | ATOM | 305 | CB  | THR | A | 41 | -3.511 | 33.892 | 44.402 | 1.00 | 55.44 |
|    | ATOM | 306 | OG1 | THR | A | 41 | -3.604 | 34.885 | 43.418 | 1.00 | 55.57 |
|    | ATOM | 307 | CG2 | THR | A | 41 | -3.872 | 32.544 | 43.802 | 1.00 | 47.78 |
|    | ATOM | 308 | N   | VAL | A | 42 | -5.755 | 32.688 | 46.848 | 1.00 | 33.25 |
|    | ATOM | 309 | CA  | VAL | A | 42 | -5.946 | 31.720 | 47.893 | 1.00 | 32.21 |
|    | ATOM | 310 | C   | VAL | A | 42 | -6.166 | 30.312 | 47.380 | 1.00 | 40.56 |



|    |      |     |     |     |   |    |         |        |        |      |       |
|----|------|-----|-----|-----|---|----|---------|--------|--------|------|-------|
|    | ATOM | 311 | O   | VAL | A | 42 | -6.827  | 30.105 | 46.376 | 1.00 | 42.56 |
|    | ATOM | 312 | CB  | VAL | A | 42 | -7.017  | 32.153 | 48.920 | 1.00 | 36.45 |
|    | ATOM | 313 | CG1 | VAL | A | 42 | -6.817  | 31.451 | 50.266 | 1.00 | 36.89 |
| 5  | ATOM | 314 | CG2 | VAL | A | 42 | -6.963  | 33.665 | 49.170 | 1.00 | 36.10 |
|    | ATOM | 315 | N   | GLN | A | 43 | -5.590  | 29.357 | 48.117 | 1.00 | 35.91 |
|    | ATOM | 316 | CA  | GLN | A | 43 | -5.678  | 27.945 | 47.838 | 1.00 | 31.59 |
|    | ATOM | 317 | C   | GLN | A | 43 | -6.346  | 27.244 | 48.988 | 1.00 | 38.98 |
|    | ATOM | 318 | O   | GLN | A | 43 | -5.916  | 27.317 | 50.144 | 1.00 | 40.92 |
| 10 | ATOM | 319 | CB  | GLN | A | 43 | -4.305  | 27.319 | 47.568 | 1.00 | 30.50 |
|    | ATOM | 320 | CG  | GLN | A | 43 | -4.362  | 25.800 | 47.259 | 1.00 | 53.80 |
|    | ATOM | 321 | CD  | GLN | A | 43 | -2.986  | 25.177 | 47.099 | 1.00 | 62.47 |
|    | ATOM | 322 | OE1 | GLN | A | 43 | -2.569  | 24.842 | 45.978 | 1.00 | 57.34 |
|    | ATOM | 323 | NE2 | GLN | A | 43 | -2.274  | 25.037 | 48.224 | 1.00 | 43.72 |
| 15 | ATOM | 324 | N   | SER | A | 44 | -7.423  | 26.555 | 48.664 | 1.00 | 33.83 |
|    | ATOM | 325 | CA  | SER | A | 44 | -8.166  | 25.839 | 49.678 | 1.00 | 31.38 |
|    | ATOM | 326 | C   | SER | A | 44 | -7.495  | 24.557 | 50.117 | 1.00 | 42.10 |
|    | ATOM | 327 | O   | SER | A | 44 | -6.955  | 23.814 | 49.292 | 1.00 | 42.78 |
|    | ATOM | 328 | CB  | SER | A | 44 | -9.576  | 25.530 | 49.226 | 1.00 | 28.60 |
| 20 | ATOM | 329 | OG  | SER | A | 44 | -10.234 | 24.785 | 50.224 | 1.00 | 34.57 |
|    | ATOM | 330 | N   | GLN | A | 45 | -7.579  | 24.286 | 51.423 | 1.00 | 38.84 |
|    | ATOM | 331 | CA  | GLN | A | 45 | -7.007  | 23.082 | 51.994 | 1.00 | 37.05 |
|    | ATOM | 332 | C   | GLN | A | 45 | -8.082  | 22.050 | 52.269 | 1.00 | 47.57 |
|    | ATOM | 333 | O   | GLN | A | 45 | -7.801  | 20.917 | 52.678 | 1.00 | 42.94 |
| 25 | ATOM | 334 | CB  | GLN | A | 45 | -6.247  | 23.411 | 53.280 | 1.00 | 36.10 |
|    | ATOM | 335 | CG  | GLN | A | 45 | -5.246  | 24.539 | 53.034 | 1.00 | 54.73 |
|    | ATOM | 336 | CD  | GLN | A | 45 | -4.323  | 24.206 | 51.888 | 1.00 | 45.43 |
|    | ATOM | 337 | OE1 | GLN | A | 45 | -4.257  | 24.888 | 50.833 | 1.00 | 39.23 |
|    | ATOM | 338 | NE2 | GLN | A | 45 | -3.621  | 23.121 | 52.092 | 1.00 | 29.80 |
| 30 | ATOM | 339 | N   | GLU | A | 46 | -9.330  | 22.459 | 52.048 | 1.00 | 50.54 |
|    | ATOM | 340 | CA  | GLU | A | 46 | -10.454 | 21.573 | 52.283 | 1.00 | 50.99 |
|    | ATOM | 341 | C   | GLU | A | 46 | -11.496 | 21.583 | 51.179 | 1.00 | 54.49 |
|    | ATOM | 342 | O   | GLU | A | 46 | -11.518 | 22.406 | 50.261 | 1.00 | 54.00 |
|    | ATOM | 343 | CB  | GLU | A | 46 | -11.139 | 21.793 | 53.657 | 1.00 | 51.61 |
| 35 | ATOM | 344 | CG  | GLU | A | 46 | -10.581 | 22.979 | 54.454 | 1.00 | 55.93 |
|    | ATOM | 345 | CD  | GLU | A | 46 | -11.427 | 23.329 | 55.646 | 1.00 | 78.67 |
|    | ATOM | 346 | OE1 | GLU | A | 46 | -12.563 | 23.765 | 55.543 | 1.00 | 69.56 |
|    | ATOM | 347 | OE2 | GLU | A | 46 | -10.814 | 23.129 | 56.796 | 1.00 | 75.10 |
|    | ATOM | 348 | N   | ASP | A | 47 | -12.387 | 20.630 | 51.300 | 1.00 | 48.90 |
| 40 | ATOM | 349 | CA  | ASP | A | 47 | -13.450 | 20.549 | 50.362 | 1.00 | 49.03 |
|    | ATOM | 350 | C   | ASP | A | 47 | -14.591 | 21.425 | 50.846 | 1.00 | 55.15 |
|    | ATOM | 351 | O   | ASP | A | 47 | -14.760 | 21.631 | 52.044 | 1.00 | 56.66 |
|    | ATOM | 352 | CB  | ASP | A | 47 | -13.913 | 19.099 | 50.227 | 1.00 | 50.20 |
|    | ATOM | 353 | CG  | ASP | A | 47 | -13.083 | 18.376 | 49.218 | 1.00 | 66.88 |
| 45 | ATOM | 354 | OD1 | ASP | A | 47 | -12.340 | 18.945 | 48.434 | 1.00 | 66.27 |
|    | ATOM | 355 | OD2 | ASP | A | 47 | -13.235 | 17.081 | 49.284 | 1.00 | 76.37 |
|    | ATOM | 356 | N   | ASN | A | 48 | -15.391 | 21.941 | 49.929 | 1.00 | 50.25 |
|    | ATOM | 357 | CA  | ASN | A | 48 | -16.519 | 22.755 | 50.339 | 1.00 | 48.45 |
|    | ATOM | 358 | C   | ASN | A | 48 | -16.115 | 24.000 | 51.115 | 1.00 | 43.07 |
| 50 | ATOM | 359 | O   | ASN | A | 48 | -16.699 | 24.351 | 52.138 | 1.00 | 39.78 |
|    | ATOM | 360 | CB  | ASN | A | 48 | -17.559 | 21.909 | 51.117 | 1.00 | 51.19 |
|    | ATOM | 361 | CG  | ASN | A | 48 | -18.985 | 22.417 | 51.005 | 1.00 | 76.39 |
|    | ATOM | 362 | OD1 | ASN | A | 48 | -19.594 | 22.348 | 49.929 | 1.00 | 85.15 |
|    | ATOM | 363 | ND2 | ASN | A | 48 | -19.515 | 22.928 | 52.115 | 1.00 | 68.29 |
| 55 | ATOM | 364 | N   | LEU | A | 49 | -15.113 | 24.688 | 50.628 | 1.00 | 35.36 |
|    | ATOM | 365 | CA  | LEU | A | 49 | -14.728 | 25.874 | 51.335 | 1.00 | 34.40 |
|    | ATOM | 366 | C   | LEU | A | 49 | -15.601 | 27.009 | 50.851 | 1.00 | 47.38 |
|    | ATOM | 367 | O   | LEU | A | 49 | -15.421 | 27.515 | 49.734 | 1.00 | 45.47 |
|    | ATOM | 368 | CB  | LEU | A | 49 | -13.239 | 26.152 | 51.173 | 1.00 | 31.04 |
| 60 | ATOM | 369 | CG  | LEU | A | 49 | -12.781 | 27.394 | 51.885 | 1.00 | 29.82 |
|    | ATOM | 370 | CD1 | LEU | A | 49 | -12.725 | 27.137 | 53.385 | 1.00 | 28.15 |
|    | ATOM | 371 | CD2 | LEU | A | 49 | -11.394 | 27.753 | 51.368 | 1.00 | 30.24 |
|    | ATOM | 372 | N   | ARG | A | 50 | -16.568 | 27.363 | 51.699 | 1.00 | 50.49 |
|    | ATOM | 373 | CA  | ARG | A | 50 | -17.560 | 28.392 | 51.401 | 1.00 | 52.83 |
|    | ATOM | 374 | C   | ARG | A | 50 | -17.169 | 29.838 | 51.702 | 1.00 | 55.57 |



|    |      |     |     |     |   |    |         |        |        |      |        |
|----|------|-----|-----|-----|---|----|---------|--------|--------|------|--------|
|    | ATOM | 375 | O   | ARG | A | 50 | -17.627 | 30.760 | 51.011 | 1.00 | 53.89  |
|    | ATOM | 376 | CB  | ARG | A | 50 | -18.928 | 28.028 | 51.986 | 1.00 | 58.35  |
|    | ATOM | 377 | CG  | ARG | A | 50 | -19.863 | 27.354 | 50.980 | 1.00 | 74.76  |
| 5  | ATOM | 378 | CD  | ARG | A | 50 | -20.438 | 26.024 | 51.462 | 1.00 | 81.60  |
|    | ATOM | 379 | NE  | ARG | A | 50 | -21.214 | 25.355 | 50.415 | 1.00 | 94.37  |
|    | ATOM | 380 | CZ  | ARG | A | 50 | -22.465 | 24.888 | 50.538 | 1.00 | 100.00 |
|    | ATOM | 381 | NH1 | ARG | A | 50 | -23.151 | 24.990 | 51.687 | 1.00 | 100.00 |
|    | ATOM | 382 | NH2 | ARG | A | 50 | -23.046 | 24.297 | 49.471 | 1.00 | 74.34  |
| 10 | ATOM | 383 | N   | SER | A | 51 | -16.331 | 30.006 | 52.743 | 1.00 | 54.71  |
|    | ATOM | 384 | CA  | SER | A | 51 | -15.823 | 31.297 | 53.224 | 1.00 | 53.49  |
|    | ATOM | 385 | C   | SER | A | 51 | -14.495 | 31.156 | 53.955 | 1.00 | 53.57  |
|    | ATOM | 386 | O   | SER | A | 51 | -14.146 | 30.062 | 54.420 | 1.00 | 52.93  |
|    | ATOM | 387 | CB  | SER | A | 51 | -16.788 | 31.900 | 54.232 | 1.00 | 54.03  |
|    | ATOM | 388 | OG  | SER | A | 51 | -16.871 | 31.048 | 55.373 | 1.00 | 45.15  |
| 15 | ATOM | 389 | N   | LEU | A | 52 | -13.796 | 32.298 | 54.067 | 1.00 | 47.19  |
|    | ATOM | 390 | CA  | LEU | A | 52 | -12.519 | 32.422 | 54.762 | 1.00 | 45.66  |
|    | ATOM | 391 | C   | LEU | A | 52 | -12.415 | 33.671 | 55.640 | 1.00 | 50.43  |
|    | ATOM | 392 | O   | LEU | A | 52 | -13.145 | 34.633 | 55.471 | 1.00 | 52.64  |
| 20 | ATOM | 393 | CB  | LEU | A | 52 | -11.235 | 32.117 | 53.923 | 1.00 | 44.20  |
|    | ATOM | 394 | CG  | LEU | A | 52 | -10.896 | 33.044 | 52.745 | 1.00 | 43.98  |
|    | ATOM | 395 | CD1 | LEU | A | 52 | -11.739 | 32.687 | 51.554 | 1.00 | 42.82  |
|    | ATOM | 396 | CD2 | LEU | A | 52 | -11.128 | 34.501 | 53.094 | 1.00 | 44.71  |
|    | ATOM | 397 | N   | VAL | A | 53 | -11.483 | 33.658 | 56.579 | 1.00 | 44.97  |
| 25 | ATOM | 398 | CA  | VAL | A | 53 | -11.271 | 34.781 | 57.455 | 1.00 | 41.69  |
|    | ATOM | 399 | C   | VAL | A | 53 | -9.859  | 35.309 | 57.339 | 1.00 | 44.25  |
|    | ATOM | 400 | O   | VAL | A | 53 | -8.866  | 34.551 | 57.302 | 1.00 | 45.42  |
|    | ATOM | 401 | CB  | VAL | A | 53 | -11.565 | 34.420 | 58.906 | 1.00 | 45.48  |
|    | ATOM | 402 | CG1 | VAL | A | 53 | -11.223 | 35.554 | 59.853 | 1.00 | 44.94  |
| 30 | ATOM | 403 | CG2 | VAL | A | 53 | -13.030 | 34.073 | 59.050 | 1.00 | 45.79  |
|    | ATOM | 404 | N   | LEU | A | 54 | -9.796  | 36.627 | 57.166 | 1.00 | 35.12  |
|    | ATOM | 405 | CA  | LEU | A | 54 | -8.555  | 37.333 | 57.080 | 1.00 | 34.14  |
|    | ATOM | 406 | C   | LEU | A | 54 | -8.377  | 38.207 | 58.326 | 1.00 | 38.92  |
|    | ATOM | 407 | O   | LEU | A | 54 | -9.281  | 38.457 | 59.108 | 1.00 | 37.45  |
| 35 | ATOM | 408 | CB  | LEU | A | 54 | -8.461  | 38.216 | 55.831 | 1.00 | 34.73  |
|    | ATOM | 409 | CG  | LEU | A | 54 | -8.539  | 37.469 | 54.510 | 1.00 | 40.25  |
|    | ATOM | 410 | CD1 | LEU | A | 54 | -8.416  | 38.488 | 53.374 | 1.00 | 40.69  |
|    | ATOM | 411 | CD2 | LEU | A | 54 | -7.424  | 36.428 | 54.415 | 1.00 | 39.64  |
|    | ATOM | 412 | N   | ASP | A | 55 | -7.192  | 38.674 | 58.524 | 1.00 | 35.02  |
| 40 | ATOM | 413 | CA  | ASP | A | 55 | -6.918  | 39.526 | 59.627 | 1.00 | 31.65  |
|    | ATOM | 414 | C   | ASP | A | 55 | -6.956  | 40.941 | 59.078 | 1.00 | 40.38  |
|    | ATOM | 415 | O   | ASP | A | 55 | -6.754  | 41.151 | 57.886 | 1.00 | 39.98  |
|    | ATOM | 416 | CB  | ASP | A | 55 | -5.494  | 39.232 | 60.075 | 1.00 | 30.92  |
|    | ATOM | 417 | CG  | ASP | A | 55 | -5.397  | 38.103 | 61.037 | 1.00 | 35.96  |
| 45 | ATOM | 418 | OD1 | ASP | A | 55 | -6.049  | 38.074 | 62.066 | 1.00 | 38.49  |
|    | ATOM | 419 | OD2 | ASP | A | 55 | -4.491  | 37.205 | 60.682 | 1.00 | 36.53  |
|    | ATOM | 420 | N   | THR | A | 56 | -7.196  | 41.900 | 59.963 | 1.00 | 42.93  |
|    | ATOM | 421 | CA  | THR | A | 56 | -7.243  | 43.334 | 59.661 | 1.00 | 41.75  |
|    | ATOM | 422 | C   | THR | A | 56 | -7.101  | 44.128 | 60.967 | 1.00 | 37.46  |
| 50 | ATOM | 423 | O   | THR | A | 56 | -7.517  | 43.687 | 62.049 | 1.00 | 36.98  |
|    | ATOM | 424 | CB  | THR | A | 56 | -8.514  | 43.825 | 58.894 | 1.00 | 37.17  |
|    | ATOM | 425 | OG1 | THR | A | 56 | -9.587  | 43.957 | 59.805 | 1.00 | 31.84  |
|    | ATOM | 426 | CG2 | THR | A | 56 | -8.910  | 42.943 | 57.714 | 1.00 | 33.58  |
|    | ATOM | 427 | N   | LYS | A | 57 | -6.513  | 45.304 | 60.863 | 1.00 | 26.63  |
| 55 | ATOM | 428 | CA  | LYS | A | 57 | -6.363  | 46.134 | 62.020 | 1.00 | 25.64  |
|    | ATOM | 429 | C   | LYS | A | 57 | -6.585  | 47.539 | 61.547 | 1.00 | 30.08  |
|    | ATOM | 430 | O   | LYS | A | 57 | -5.854  | 48.012 | 60.711 | 1.00 | 25.68  |
|    | ATOM | 431 | CB  | LYS | A | 57 | -4.991  | 45.983 | 62.641 | 1.00 | 27.34  |
|    | ATOM | 432 | CG  | LYS | A | 57 | -4.907  | 46.387 | 64.100 | 1.00 | 35.83  |
| 60 | ATOM | 433 | CD  | LYS | A | 57 | -3.514  | 46.904 | 64.471 | 1.00 | 35.57  |
|    | ATOM | 434 | CE  | LYS | A | 57 | -2.901  | 46.225 | 65.689 | 1.00 | 50.54  |
|    | ATOM | 435 | NZ  | LYS | A | 57 | -2.521  | 47.180 | 66.757 | 1.00 | 55.43  |
|    | ATOM | 436 | N   | ASP | A | 58 | -7.617  | 48.188 | 62.065 | 1.00 | 32.68  |
|    | ATOM | 437 | CA  | ASP | A | 58 | -7.895  | 49.545 | 61.665 | 1.00 | 35.27  |
|    | ATOM | 438 | C   | ASP | A | 58 | -7.894  | 49.710 | 60.149 | 1.00 | 38.24  |



|    |      |     |     |     |   |    |         |        |        |      |        |
|----|------|-----|-----|-----|---|----|---------|--------|--------|------|--------|
|    | ATOM | 439 | O   | ASP | A | 58 | -7.289  | 50.627 | 59.571 | 1.00 | 35.86  |
|    | ATOM | 440 | CB  | ASP | A | 58 | -6.968  | 50.550 | 62.386 | 1.00 | 37.22  |
|    | ATOM | 441 | CG  | ASP | A | 58 | -7.041  | 50.393 | 63.880 | 1.00 | 50.71  |
| 5  | ATOM | 442 | OD1 | ASP | A | 58 | -8.073  | 50.136 | 64.478 | 1.00 | 57.20  |
|    | ATOM | 443 | OD2 | ASP | A | 58 | -5.878  | 50.562 | 64.463 | 1.00 | 45.82  |
|    | ATOM | 444 | N   | LEU | A | 59 | -8.604  | 48.796 | 59.516 | 1.00 | 37.68  |
|    | ATOM | 445 | CA  | LEU | A | 59 | -8.720  | 48.813 | 58.079 | 1.00 | 39.36  |
|    | ATOM | 446 | C   | LEU | A | 59 | -10.077 | 49.243 | 57.555 | 1.00 | 45.51  |
| 10 | ATOM | 447 | O   | LEU | A | 59 | -11.146 | 48.946 | 58.120 | 1.00 | 44.18  |
|    | ATOM | 448 | CB  | LEU | A | 59 | -8.265  | 47.506 | 57.422 | 1.00 | 38.42  |
|    | ATOM | 449 | CG  | LEU | A | 59 | -6.762  | 47.475 | 57.218 | 1.00 | 37.40  |
|    | ATOM | 450 | CD1 | LEU | A | 59 | -6.392  | 46.173 | 56.526 | 1.00 | 36.39  |
|    | ATOM | 451 | CD2 | LEU | A | 59 | -6.321  | 48.655 | 56.361 | 1.00 | 36.57  |
| 15 | ATOM | 452 | N   | THR | A | 60 | -9.984  | 49.949 | 56.437 | 1.00 | 42.59  |
|    | ATOM | 453 | CA  | THR | A | 60 | -11.132 | 50.483 | 55.734 | 1.00 | 42.63  |
|    | ATOM | 454 | C   | THR | A | 60 | -11.357 | 49.705 | 54.463 | 1.00 | 38.18  |
|    | ATOM | 455 | O   | THR | A | 60 | -10.632 | 49.856 | 53.454 | 1.00 | 34.33  |
|    | ATOM | 456 | CB  | THR | A | 60 | -11.030 | 52.028 | 55.532 | 1.00 | 65.15  |
| 20 | ATOM | 457 | OG1 | THR | A | 60 | -11.806 | 52.736 | 56.504 | 1.00 | 67.56  |
|    | ATOM | 458 | CG2 | THR | A | 60 | -11.345 | 52.480 | 54.104 | 1.00 | 56.89  |
|    | ATOM | 459 | N   | ILE | A | 61 | -12.360 | 48.847 | 54.571 | 1.00 | 33.39  |
|    | ATOM | 460 | CA  | ILE | A | 61 | -12.753 | 47.975 | 53.482 | 1.00 | 35.89  |
|    | ATOM | 461 | C   | ILE | A | 61 | -13.726 | 48.634 | 52.533 | 1.00 | 41.05  |
| 25 | ATOM | 462 | O   | ILE | A | 61 | -14.913 | 48.706 | 52.840 | 1.00 | 40.08  |
|    | ATOM | 463 | CB  | ILE | A | 61 | -13.403 | 46.670 | 53.944 | 1.00 | 39.71  |
|    | ATOM | 464 | CG1 | ILE | A | 61 | -12.482 | 45.826 | 54.832 | 1.00 | 39.90  |
|    | ATOM | 465 | CG2 | ILE | A | 61 | -13.788 | 45.900 | 52.691 | 1.00 | 38.96  |
|    | ATOM | 466 | CD1 | ILE | A | 61 | -11.027 | 45.851 | 54.358 | 1.00 | 49.61  |
| 30 | ATOM | 467 | N   | GLU | A | 62 | -13.219 | 49.080 | 51.391 | 1.00 | 40.23  |
|    | ATOM | 468 | CA  | GLU | A | 62 | -14.040 | 49.700 | 50.365 | 1.00 | 41.73  |
|    | ATOM | 469 | C   | GLU | A | 62 | -14.986 | 48.633 | 49.826 | 1.00 | 47.09  |
|    | ATOM | 470 | O   | GLU | A | 62 | -16.207 | 48.726 | 49.926 | 1.00 | 47.52  |
|    | ATOM | 471 | CB  | GLU | A | 62 | -13.138 | 50.272 | 49.239 | 1.00 | 44.08  |
| 35 | ATOM | 472 | CG  | GLU | A | 62 | -13.765 | 51.406 | 48.381 | 1.00 | 64.08  |
|    | ATOM | 473 | CD  | GLU | A | 62 | -14.686 | 50.946 | 47.256 | 1.00 | 100.00 |
|    | ATOM | 474 | OE1 | GLU | A | 62 | -15.458 | 50.002 | 47.376 | 1.00 | 100.00 |
|    | ATOM | 475 | OE2 | GLU | A | 62 | -14.591 | 51.670 | 46.146 | 1.00 | 75.11  |
|    | ATOM | 476 | N   | LYS | A | 63 | -14.399 | 47.580 | 49.267 | 1.00 | 43.46  |
| 40 | ATOM | 477 | CA  | LYS | A | 63 | -15.168 | 46.474 | 48.746 | 1.00 | 40.53  |
|    | ATOM | 478 | C   | LYS | A | 63 | -14.250 | 45.307 | 48.489 | 1.00 | 45.38  |
|    | ATOM | 479 | O   | LYS | A | 63 | -13.046 | 45.500 | 48.362 | 1.00 | 43.51  |
|    | ATOM | 480 | CB  | LYS | A | 63 | -15.818 | 46.830 | 47.428 | 1.00 | 40.46  |
|    | ATOM | 481 | CG  | LYS | A | 63 | -14.789 | 46.959 | 46.321 | 1.00 | 20.53  |
| 45 | ATOM | 482 | CD  | LYS | A | 63 | -15.367 | 47.555 | 45.054 | 1.00 | 28.36  |
|    | ATOM | 483 | CE  | LYS | A | 63 | -14.315 | 48.158 | 44.139 | 1.00 | 40.61  |
|    | ATOM | 484 | NZ  | LYS | A | 63 | -14.588 | 47.938 | 42.711 | 1.00 | 54.71  |
|    | ATOM | 485 | N   | VAL | A | 64 | -14.862 | 44.116 | 48.441 | 1.00 | 45.57  |
|    | ATOM | 486 | CA  | VAL | A | 64 | -14.190 | 42.844 | 48.171 | 1.00 | 44.90  |
| 50 | ATOM | 487 | C   | VAL | A | 64 | -14.666 | 42.263 | 46.841 | 1.00 | 46.44  |
|    | ATOM | 488 | O   | VAL | A | 64 | -15.826 | 41.917 | 46.700 | 1.00 | 45.81  |
|    | ATOM | 489 | CB  | VAL | A | 64 | -14.505 | 41.748 | 49.192 | 1.00 | 46.24  |
|    | ATOM | 490 | CG1 | VAL | A | 64 | -13.864 | 40.471 | 48.669 | 1.00 | 44.81  |
|    | ATOM | 491 | CG2 | VAL | A | 64 | -14.040 | 42.048 | 50.627 | 1.00 | 44.77  |
| 55 | ATOM | 492 | N   | VAL | A | 65 | -13.793 | 42.099 | 45.875 | 1.00 | 43.10  |
|    | ATOM | 493 | CA  | VAL | A | 65 | -14.240 | 41.537 | 44.604 | 1.00 | 41.42  |
|    | ATOM | 494 | C   | VAL | A | 65 | -13.707 | 40.156 | 44.282 | 1.00 | 42.13  |
|    | ATOM | 495 | O   | VAL | A | 65 | -12.605 | 39.787 | 44.660 | 1.00 | 42.64  |
|    | ATOM | 496 | CB  | VAL | A | 65 | -13.856 | 42.462 | 43.484 | 1.00 | 44.58  |
| 60 | ATOM | 497 | CG1 | VAL | A | 65 | -14.520 | 42.037 | 42.189 | 1.00 | 42.79  |
|    | ATOM | 498 | CG2 | VAL | A | 65 | -14.264 | 43.874 | 43.883 | 1.00 | 45.05  |
|    | ATOM | 499 | N   | ILE | A | 66 | -14.515 | 39.402 | 43.556 | 1.00 | 38.68  |
|    | ATOM | 500 | CA  | ILE | A | 66 | -14.179 | 38.053 | 43.113 | 1.00 | 39.98  |
|    | ATOM | 501 | C   | ILE | A | 66 | -14.899 | 37.774 | 41.802 | 1.00 | 44.86  |
|    | ATOM | 502 | O   | ILE | A | 66 | -16.136 | 37.735 | 41.729 | 1.00 | 42.69  |



|    |      |     |     |     |   |    |         |        |        |      |        |
|----|------|-----|-----|-----|---|----|---------|--------|--------|------|--------|
|    | ATOM | 503 | CB  | ILE | A | 66 | -14.520 | 36.947 | 44.113 | 1.00 | 44.28  |
|    | ATOM | 504 | CG1 | ILE | A | 66 | -13.813 | 37.127 | 45.445 | 1.00 | 47.27  |
|    | ATOM | 505 | CG2 | ILE | A | 66 | -14.141 | 35.578 | 43.550 | 1.00 | 42.84  |
| 5  | ATOM | 506 | CD1 | ILE | A | 66 | -14.352 | 36.169 | 46.514 | 1.00 | 38.79  |
|    | ATOM | 507 | N   | ASN | A | 67 | -14.120 | 37.549 | 40.759 | 1.00 | 42.94  |
|    | ATOM | 508 | CA  | ASN | A | 67 | -14.715 | 37.266 | 39.472 | 1.00 | 44.24  |
|    | ATOM | 509 | C   | ASN | A | 67 | -15.541 | 38.444 | 39.008 | 1.00 | 54.25  |
|    | ATOM | 510 | O   | ASN | A | 67 | -16.743 | 38.344 | 38.768 | 1.00 | 57.56  |
| 10 | ATOM | 511 | CB  | ASN | A | 67 | -15.595 | 36.007 | 39.507 | 1.00 | 40.72  |
|    | ATOM | 512 | CG  | ASN | A | 67 | -14.788 | 34.759 | 39.745 | 1.00 | 57.39  |
|    | ATOM | 513 | OD1 | ASN | A | 67 | -13.581 | 34.711 | 39.454 | 1.00 | 52.63  |
|    | ATOM | 514 | ND2 | ASN | A | 67 | -15.446 | 33.760 | 40.317 | 1.00 | 44.54  |
|    | ATOM | 515 | N   | GLY | A | 68 | -14.876 | 39.574 | 38.899 | 1.00 | 50.43  |
| 15 | ATOM | 516 | CA  | GLY | A | 68 | -15.517 | 40.796 | 38.462 | 1.00 | 48.89  |
|    | ATOM | 517 | C   | GLY | A | 68 | -16.807 | 41.115 | 39.194 | 1.00 | 48.77  |
|    | ATOM | 518 | O   | GLY | A | 68 | -17.523 | 42.018 | 38.803 | 1.00 | 51.39  |
|    | ATOM | 519 | N   | GLN | A | 69 | -17.129 | 40.385 | 40.244 | 1.00 | 40.06  |
|    | ATOM | 520 | CA  | GLN | A | 69 | -18.348 | 40.716 | 40.928 | 1.00 | 40.02  |
| 20 | ATOM | 521 | C   | GLN | A | 69 | -18.031 | 41.059 | 42.364 | 1.00 | 50.45  |
|    | ATOM | 522 | O   | GLN | A | 69 | -16.943 | 40.748 | 42.855 | 1.00 | 50.53  |
|    | ATOM | 523 | CB  | GLN | A | 69 | -19.415 | 39.602 | 40.829 | 1.00 | 40.78  |
|    | ATOM | 524 | CG  | GLN | A | 69 | -19.966 | 39.367 | 39.414 | 1.00 | 23.77  |
|    | ATOM | 525 | CD  | GLN | A | 69 | -20.513 | 40.646 | 38.831 | 1.00 | 56.53  |
| 25 | ATOM | 526 | OE1 | GLN | A | 69 | -19.974 | 41.198 | 37.859 | 1.00 | 55.28  |
|    | ATOM | 527 | NE2 | GLN | A | 69 | -21.588 | 41.134 | 39.437 | 1.00 | 62.26  |
|    | ATOM | 528 | N   | GLU | A | 70 | -18.975 | 41.718 | 43.028 | 1.00 | 49.43  |
|    | ATOM | 529 | CA  | GLU | A | 70 | -18.766 | 42.094 | 44.407 | 1.00 | 50.67  |
|    | ATOM | 530 | C   | GLU | A | 70 | -19.296 | 40.996 | 45.288 | 1.00 | 57.90  |
| 30 | ATOM | 531 | O   | GLU | A | 70 | -20.272 | 40.367 | 44.909 | 1.00 | 63.90  |
|    | ATOM | 532 | CB  | GLU | A | 70 | -19.449 | 43.434 | 44.732 | 1.00 | 52.26  |
|    | ATOM | 533 | CG  | GLU | A | 70 | -18.824 | 44.624 | 43.970 | 1.00 | 64.80  |
|    | ATOM | 534 | CD  | GLU | A | 70 | -19.181 | 45.967 | 44.555 | 1.00 | 91.82  |
|    | ATOM | 535 | OE1 | GLU | A | 70 | -19.749 | 46.108 | 45.629 | 1.00 | 100.00 |
| 35 | ATOM | 536 | OE2 | GLU | A | 70 | -18.814 | 46.963 | 43.785 | 1.00 | 76.01  |
|    | ATOM | 537 | N   | VAL | A | 71 | -18.655 | 40.742 | 46.433 | 1.00 | 47.28  |
|    | ATOM | 538 | CA  | VAL | A | 71 | -19.119 | 39.685 | 47.335 | 1.00 | 43.84  |
|    | ATOM | 539 | C   | VAL | A | 71 | -19.434 | 40.153 | 48.768 | 1.00 | 41.62  |
|    | ATOM | 540 | O   | VAL | A | 71 | -18.983 | 41.206 | 49.254 | 1.00 | 35.70  |
| 40 | ATOM | 541 | CB  | VAL | A | 71 | -18.308 | 38.361 | 47.273 | 1.00 | 46.05  |
|    | ATOM | 542 | CG1 | VAL | A | 71 | -18.062 | 37.923 | 45.827 | 1.00 | 45.19  |
|    | ATOM | 543 | CG2 | VAL | A | 71 | -16.979 | 38.460 | 48.017 | 1.00 | 45.24  |
|    | ATOM | 544 | N   | LYS | A | 72 | -20.239 | 39.343 | 49.431 | 1.00 | 39.34  |
|    | ATOM | 545 | CA  | LYS | A | 72 | -20.610 | 39.594 | 50.792 | 1.00 | 42.40  |
| 45 | ATOM | 546 | C   | LYS | A | 72 | -19.347 | 39.466 | 51.668 | 1.00 | 56.92  |
|    | ATOM | 547 | O   | LYS | A | 72 | -18.399 | 38.729 | 51.334 | 1.00 | 59.27  |
|    | ATOM | 548 | CB  | LYS | A | 72 | -21.719 | 38.629 | 51.211 | 1.00 | 45.76  |
|    | ATOM | 549 | CG  | LYS | A | 72 | -22.378 | 38.960 | 52.557 | 1.00 | 86.98  |
|    | ATOM | 550 | CD  | LYS | A | 72 | -23.898 | 38.767 | 52.606 | 1.00 | 100.00 |
| 50 | ATOM | 551 | CE  | LYS | A | 72 | -24.656 | 40.012 | 53.077 | 1.00 | 100.00 |
|    | ATOM | 552 | NZ  | LYS | A | 72 | -26.011 | 39.730 | 53.592 | 1.00 | 100.00 |
|    | ATOM | 553 | N   | TYR | A | 73 | -19.332 | 40.210 | 52.780 | 1.00 | 55.45  |
|    | ATOM | 554 | CA  | TYR | A | 73 | -18.236 | 40.226 | 53.747 | 1.00 | 53.31  |
|    | ATOM | 555 | C   | TYR | A | 73 | -18.636 | 40.884 | 55.068 | 1.00 | 50.87  |
| 55 | ATOM | 556 | O   | TYR | A | 73 | -19.552 | 41.703 | 55.139 | 1.00 | 47.82  |
|    | ATOM | 557 | CB  | TYR | A | 73 | -16.891 | 40.741 | 53.214 | 1.00 | 52.73  |
|    | ATOM | 558 | CG  | TYR | A | 73 | -16.765 | 42.244 | 53.227 | 1.00 | 51.76  |
|    | ATOM | 559 | CD1 | TYR | A | 73 | -16.539 | 42.946 | 54.416 | 1.00 | 52.82  |
|    | ATOM | 560 | CD2 | TYR | A | 73 | -16.927 | 42.967 | 52.039 | 1.00 | 53.30  |
| 60 | ATOM | 561 | CE1 | TYR | A | 73 | -16.439 | 44.340 | 54.422 | 1.00 | 52.71  |
|    | ATOM | 562 | CE2 | TYR | A | 73 | -16.804 | 44.359 | 52.026 | 1.00 | 55.39  |
|    | ATOM | 563 | CZ  | TYR | A | 73 | -16.592 | 45.044 | 53.229 | 1.00 | 63.45  |
|    | ATOM | 564 | OH  | TYR | A | 73 | -16.471 | 46.404 | 53.215 | 1.00 | 69.53  |
|    | ATOM | 565 | N   | ALA | A | 74 | -17.927 | 40.494 | 56.112 | 1.00 | 45.37  |
|    | ATOM | 566 | CA  | ALA | A | 74 | -18.180 | 40.999 | 57.433 | 1.00 | 42.62  |



|    |      |     |     |     |   |    |         |        |        |      |        |
|----|------|-----|-----|-----|---|----|---------|--------|--------|------|--------|
|    | ATOM | 567 | C   | ALA | A | 74 | -16.892 | 41.265 | 58.222 | 1.00 | 47.81  |
|    | ATOM | 568 | O   | ALA | A | 74 | -15.894 | 40.554 | 58.133 | 1.00 | 45.50  |
|    | ATOM | 569 | CB  | ALA | A | 74 | -19.111 | 40.035 | 58.170 | 1.00 | 40.75  |
| 5  | ATOM | 570 | N   | LEU | A | 75 | -16.930 | 42.323 | 59.005 | 1.00 | 49.02  |
|    | ATOM | 571 | CA  | LEU | A | 75 | -15.829 | 42.693 | 59.869 | 1.00 | 48.85  |
|    | ATOM | 572 | C   | LEU | A | 75 | -16.319 | 42.464 | 61.281 | 1.00 | 47.18  |
|    | ATOM | 573 | O   | LEU | A | 75 | -17.309 | 43.021 | 61.687 | 1.00 | 44.35  |
|    | ATOM | 574 | CB  | LEU | A | 75 | -15.332 | 44.136 | 59.675 | 1.00 | 49.64  |
| 10 | ATOM | 575 | CG  | LEU | A | 75 | -14.789 | 44.357 | 58.270 | 1.00 | 58.09  |
|    | ATOM | 576 | CD1 | LEU | A | 75 | -14.524 | 45.841 | 58.023 | 1.00 | 61.34  |
|    | ATOM | 577 | CD2 | LEU | A | 75 | -13.512 | 43.565 | 58.069 | 1.00 | 62.34  |
|    | ATOM | 578 | N   | GLY | A | 76 | -15.647 | 41.592 | 62.004 | 1.00 | 47.67  |
|    | ATOM | 579 | CA  | GLY | A | 76 | -16.034 | 41.281 | 63.359 | 1.00 | 46.79  |
| 15 | ATOM | 580 | C   | GLY | A | 76 | -15.495 | 42.337 | 64.279 | 1.00 | 47.74  |
|    | ATOM | 581 | O   | GLY | A | 76 | -14.656 | 43.171 | 63.882 | 1.00 | 42.87  |
|    | ATOM | 582 | N   | GLU | A | 77 | -15.988 | 42.311 | 65.502 | 1.00 | 48.32  |
|    | ATOM | 583 | CA  | GLU | A | 77 | -15.526 | 43.300 | 66.431 | 1.00 | 52.14  |
|    | ATOM | 584 | C   | GLU | A | 77 | -14.029 | 43.195 | 66.679 | 1.00 | 56.71  |
| 20 | ATOM | 585 | O   | GLU | A | 77 | -13.418 | 42.120 | 66.591 | 1.00 | 55.78  |
|    | ATOM | 586 | CB  | GLU | A | 77 | -16.357 | 43.341 | 67.732 | 1.00 | 55.55  |
|    | ATOM | 587 | CG  | GLU | A | 77 | -17.198 | 42.063 | 67.969 | 1.00 | 79.57  |
|    | ATOM | 588 | CD  | GLU | A | 77 | -17.440 | 41.739 | 69.427 | 1.00 | 100.00 |
|    | ATOM | 589 | OE1 | GLU | A | 77 | -16.537 | 41.435 | 70.211 | 1.00 | 100.00 |
| 25 | ATOM | 590 | OE2 | GLU | A | 77 | -18.712 | 41.799 | 69.770 | 1.00 | 100.00 |
|    | ATOM | 591 | N   | ARG | A | 78 | -13.452 | 44.344 | 67.000 | 1.00 | 54.17  |
|    | ATOM | 592 | CA  | ARG | A | 78 | -12.041 | 44.433 | 67.298 | 1.00 | 53.38  |
|    | ATOM | 593 | C   | ARG | A | 78 | -11.627 | 43.656 | 68.579 | 1.00 | 58.88  |
|    | ATOM | 594 | O   | ARG | A | 78 | -12.247 | 43.767 | 69.635 | 1.00 | 61.35  |
| 30 | ATOM | 595 | CB  | ARG | A | 78 | -11.571 | 45.891 | 67.367 | 1.00 | 41.96  |
|    | ATOM | 596 | CG  | ARG | A | 78 | -10.050 | 46.006 | 67.326 | 1.00 | 38.20  |
|    | ATOM | 597 | CD  | ARG | A | 78 | -9.537  | 47.411 | 67.551 | 1.00 | 44.73  |
|    | ATOM | 598 | NE  | ARG | A | 78 | -8.294  | 47.648 | 66.842 | 1.00 | 66.47  |
|    | ATOM | 599 | CZ  | ARG | A | 78 | -7.250  | 48.247 | 67.389 | 1.00 | 97.61  |
| 35 | ATOM | 600 | NH1 | ARG | A | 78 | -7.276  | 48.692 | 68.645 | 1.00 | 100.00 |
|    | ATOM | 601 | NH2 | ARG | A | 78 | -6.151  | 48.413 | 66.663 | 1.00 | 80.10  |
|    | ATOM | 602 | N   | GLN | A | 79 | -10.557 | 42.857 | 68.463 | 1.00 | 49.54  |
|    | ATOM | 603 | CA  | GLN | A | 79 | -9.995  | 42.115 | 69.566 | 1.00 | 47.71  |
|    | ATOM | 604 | C   | GLN | A | 79 | -8.664  | 42.789 | 69.865 | 1.00 | 49.77  |
| 40 | ATOM | 605 | O   | GLN | A | 79 | -7.626  | 42.421 | 69.333 | 1.00 | 52.63  |
|    | ATOM | 606 | CB  | GLN | A | 79 | -9.803  | 40.613 | 69.240 | 1.00 | 49.05  |
|    | ATOM | 607 | CG  | GLN | A | 79 | -11.109 | 39.794 | 69.339 | 1.00 | 57.32  |
|    | ATOM | 608 | CD  | GLN | A | 79 | -11.043 | 38.435 | 68.656 | 1.00 | 69.51  |
|    | ATOM | 609 | OE1 | GLN | A | 79 | -10.400 | 37.480 | 69.152 | 1.00 | 49.72  |
| 45 | ATOM | 610 | NE2 | GLN | A | 79 | -11.727 | 38.340 | 67.517 | 1.00 | 62.60  |
|    | ATOM | 611 | N   | SER | A | 80 | -8.699  | 43.826 | 70.683 | 1.00 | 41.74  |
|    | ATOM | 612 | CA  | SER | A | 80 | -7.490  | 44.543 | 71.022 | 1.00 | 37.90  |
|    | ATOM | 613 | C   | SER | A | 80 | -6.437  | 44.559 | 69.920 | 1.00 | 35.98  |
|    | ATOM | 614 | O   | SER | A | 80 | -6.736  | 44.939 | 68.801 | 1.00 | 34.52  |
| 50 | ATOM | 615 | CB  | SER | A | 80 | -6.910  | 44.144 | 72.372 | 1.00 | 39.07  |
|    | ATOM | 616 | OG  | SER | A | 80 | -7.255  | 42.803 | 72.684 | 1.00 | 61.32  |
|    | ATOM | 617 | N   | TYR | A | 81 | -5.206  | 44.154 | 70.289 | 1.00 | 29.92  |
|    | ATOM | 618 | CA  | TYR | A | 81 | -4.027  | 44.114 | 69.430 | 1.00 | 26.45  |
|    | ATOM | 619 | C   | TYR | A | 81 | -4.163  | 43.116 | 68.285 | 1.00 | 30.82  |
| 55 | ATOM | 620 | O   | TYR | A | 81 | -3.480  | 43.215 | 67.269 | 1.00 | 34.48  |
|    | ATOM | 621 | CB  | TYR | A | 81 | -2.727  | 43.893 | 70.257 | 1.00 | 25.19  |
|    | ATOM | 622 | CG  | TYR | A | 81 | -2.713  | 42.491 | 70.839 | 1.00 | 24.57  |
|    | ATOM | 623 | CD1 | TYR | A | 81 | -3.327  | 42.247 | 72.066 | 1.00 | 27.27  |
|    | ATOM | 624 | CD2 | TYR | A | 81 | -2.165  | 41.410 | 70.148 | 1.00 | 21.82  |
| 60 | ATOM | 625 | CE1 | TYR | A | 81 | -3.380  | 40.975 | 72.632 | 1.00 | 26.49  |
|    | ATOM | 626 | CE2 | TYR | A | 81 | -2.230  | 40.122 | 70.682 | 1.00 | 23.48  |
|    | ATOM | 627 | CZ  | TYR | A | 81 | -2.827  | 39.908 | 71.930 | 1.00 | 38.28  |
|    | ATOM | 628 | OH  | TYR | A | 81 | -2.889  | 38.653 | 72.493 | 1.00 | 42.17  |
|    | ATOM | 629 | N   | LYS | A | 82 | -5.038  | 42.136 | 68.415 | 1.00 | 26.97  |
|    | ATOM | 630 | CA  | LYS | A | 82 | -5.170  | 41.229 | 67.293 | 1.00 | 27.99  |



|    |      |     |     |     |   |    |         |        |        |      |       |
|----|------|-----|-----|-----|---|----|---------|--------|--------|------|-------|
|    | ATOM | 631 | C   | LYS | A | 82 | -5.867  | 41.898 | 66.072 | 1.00 | 38.90 |
|    | ATOM | 632 | O   | LYS | A | 82 | -5.614  | 41.541 | 64.900 | 1.00 | 37.15 |
|    | ATOM | 633 | CB  | LYS | A | 82 | -5.785  | 39.918 | 67.708 | 1.00 | 27.59 |
| 5  | ATOM | 634 | CG  | LYS | A | 82 | -5.169  | 39.451 | 69.008 | 1.00 | 39.68 |
|    | ATOM | 635 | CD  | LYS | A | 82 | -5.435  | 37.993 | 69.350 | 1.00 | 46.78 |
|    | ATOM | 636 | CE  | LYS | A | 82 | -6.414  | 37.819 | 70.492 | 1.00 | 59.84 |
|    | ATOM | 637 | NZ  | LYS | A | 82 | -7.097  | 36.523 | 70.452 | 1.00 | 63.48 |
|    | ATOM | 638 | N   | GLY | A | 83 | -6.738  | 42.894 | 66.367 | 1.00 | 35.64 |
| 10 | ATOM | 639 | CA  | GLY | A | 83 | -7.512  | 43.620 | 65.368 | 1.00 | 33.65 |
|    | ATOM | 640 | C   | GLY | A | 83 | -8.866  | 42.925 | 65.111 | 1.00 | 32.95 |
|    | ATOM | 641 | O   | GLY | A | 83 | -9.297  | 42.063 | 65.870 | 1.00 | 28.28 |
|    | ATOM | 642 | N   | SER | A | 84 | -9.535  | 43.300 | 64.026 | 1.00 | 34.51 |
|    | ATOM | 643 | CA  | SER | A | 84 | -10.839 | 42.742 | 63.673 | 1.00 | 36.13 |
|    | ATOM | 644 | C   | SER | A | 84 | -10.796 | 41.724 | 62.549 | 1.00 | 40.65 |
| 15 | ATOM | 645 | O   | SER | A | 84 | -10.173 | 41.893 | 61.501 | 1.00 | 39.77 |
|    | ATOM | 646 | CB  | SER | A | 84 | -11.883 | 43.808 | 63.383 | 1.00 | 37.68 |
|    | ATOM | 647 | OG  | SER | A | 84 | -11.812 | 44.832 | 64.352 | 1.00 | 45.14 |
|    | ATOM | 648 | N   | PRO | A | 85 | -11.491 | 40.656 | 62.791 | 1.00 | 37.01 |
| 20 | ATOM | 649 | CA  | PRO | A | 85 | -11.573 | 39.559 | 61.863 | 1.00 | 34.91 |
|    | ATOM | 650 | C   | PRO | A | 85 | -12.459 | 39.946 | 60.712 | 1.00 | 35.92 |
|    | ATOM | 651 | O   | PRO | A | 85 | -13.514 | 40.522 | 60.941 | 1.00 | 35.30 |
|    | ATOM | 652 | CB  | PRO | A | 85 | -12.227 | 38.406 | 62.647 | 1.00 | 37.00 |
|    | ATOM | 653 | CG  | PRO | A | 85 | -12.714 | 38.981 | 63.974 | 1.00 | 44.97 |
| 25 | ATOM | 654 | CD  | PRO | A | 85 | -12.325 | 40.462 | 64.004 | 1.00 | 40.72 |
|    | ATOM | 655 | N   | MET | A | 86 | -12.018 | 39.642 | 59.487 | 1.00 | 30.47 |
|    | ATOM | 656 | CA  | MET | A | 86 | -12.756 | 39.960 | 58.275 | 1.00 | 28.55 |
|    | ATOM | 657 | C   | MET | A | 86 | -13.165 | 38.683 | 57.552 | 1.00 | 40.49 |
|    | ATOM | 658 | O   | MET | A | 86 | -12.338 | 38.015 | 56.954 | 1.00 | 39.69 |
| 30 | ATOM | 659 | CB  | MET | A | 86 | -11.921 | 40.829 | 57.337 | 1.00 | 29.51 |
|    | ATOM | 660 | CG  | MET | A | 86 | -12.750 | 41.242 | 56.136 | 1.00 | 37.40 |
|    | ATOM | 661 | SD  | MET | A | 86 | -11.816 | 41.878 | 54.701 | 1.00 | 47.84 |
|    | ATOM | 662 | CE  | MET | A | 86 | -13.244 | 42.527 | 53.805 | 1.00 | 46.52 |
|    | ATOM | 663 | N   | GLU | A | 87 | -14.441 | 38.324 | 57.610 | 1.00 | 44.34 |
| 35 | ATOM | 664 | CA  | GLU | A | 87 | -14.912 | 37.107 | 56.950 | 1.00 | 47.21 |
|    | ATOM | 665 | C   | GLU | A | 87 | -15.495 | 37.352 | 55.560 | 1.00 | 51.53 |
|    | ATOM | 666 | O   | GLU | A | 87 | -16.425 | 38.129 | 55.424 | 1.00 | 53.92 |
|    | ATOM | 667 | CB  | GLU | A | 87 | -15.942 | 36.390 | 57.813 | 1.00 | 49.46 |
|    | ATOM | 668 | CG  | GLU | A | 87 | -16.144 | 34.937 | 57.389 | 1.00 | 56.39 |
| 40 | ATOM | 669 | CD  | GLU | A | 87 | -17.300 | 34.316 | 58.104 | 1.00 | 80.78 |
|    | ATOM | 670 | OE1 | GLU | A | 87 | -18.439 | 34.738 | 57.994 | 1.00 | 86.69 |
|    | ATOM | 671 | OE2 | GLU | A | 87 | -16.943 | 33.301 | 58.868 | 1.00 | 68.69 |
|    | ATOM | 672 | N   | ILE | A | 88 | -14.942 | 36.659 | 54.544 | 1.00 | 43.84 |
|    | ATOM | 673 | CA  | ILE | A | 88 | -15.332 | 36.765 | 53.145 | 1.00 | 40.15 |
| 45 | ATOM | 674 | C   | ILE | A | 88 | -16.145 | 35.610 | 52.613 | 1.00 | 46.72 |
|    | ATOM | 675 | O   | ILE | A | 88 | -15.725 | 34.460 | 52.656 | 1.00 | 48.10 |
|    | ATOM | 676 | CB  | ILE | A | 88 | -14.107 | 36.891 | 52.292 | 1.00 | 39.13 |
|    | ATOM | 677 | CG1 | ILE | A | 88 | -13.328 | 38.146 | 52.696 | 1.00 | 38.40 |
|    | ATOM | 678 | CG2 | ILE | A | 88 | -14.538 | 36.932 | 50.839 | 1.00 | 28.13 |
| 50 | ATOM | 679 | CD1 | ILE | A | 88 | -11.944 | 38.200 | 52.051 | 1.00 | 30.07 |
|    | ATOM | 680 | N   | SER | A | 89 | -17.314 | 35.931 | 52.077 | 1.00 | 45.16 |
|    | ATOM | 681 | CA  | SER | A | 89 | -18.181 | 34.893 | 51.559 | 1.00 | 44.76 |
|    | ATOM | 682 | C   | SER | A | 89 | -17.902 | 34.531 | 50.131 | 1.00 | 46.01 |
|    | ATOM | 683 | O   | SER | A | 89 | -18.048 | 35.347 | 49.243 | 1.00 | 44.34 |
| 55 | ATOM | 684 | CB  | SER | A | 89 | -19.657 | 35.121 | 51.827 | 1.00 | 51.87 |
|    | ATOM | 685 | OG  | SER | A | 89 | -19.942 | 34.834 | 53.198 | 1.00 | 69.07 |
|    | ATOM | 686 | N   | LEU | A | 90 | -17.494 | 33.279 | 49.914 | 1.00 | 46.43 |
|    | ATOM | 687 | CA  | LEU | A | 90 | -17.204 | 32.804 | 48.575 | 1.00 | 46.93 |
|    | ATOM | 688 | C   | LEU | A | 90 | -18.450 | 32.235 | 47.935 | 1.00 | 55.26 |
| 60 | ATOM | 689 | O   | LEU | A | 90 | -19.210 | 31.476 | 48.556 | 1.00 | 54.94 |
|    | ATOM | 690 | CB  | LEU | A | 90 | -16.080 | 31.750 | 48.521 | 1.00 | 46.14 |
|    | ATOM | 691 | CG  | LEU | A | 90 | -15.262 | 31.607 | 49.792 | 1.00 | 50.78 |
|    | ATOM | 692 | CD1 | LEU | A | 90 | -14.546 | 30.261 | 49.806 | 1.00 | 50.27 |
|    | ATOM | 693 | CD2 | LEU | A | 90 | -14.219 | 32.708 | 49.863 | 1.00 | 55.52 |
|    | ATOM | 694 | N   | PRO | A | 91 | -18.626 | 32.607 | 46.683 | 1.00 | 54.81 |



|    |      |     |     |     |   |    |         |        |        |      |        |
|----|------|-----|-----|-----|---|----|---------|--------|--------|------|--------|
|    | ATOM | 695 | CA  | PRO | A | 91 | -19.756 | 32.183 | 45.870 | 1.00 | 58.45  |
|    | ATOM | 696 | C   | PRO | A | 91 | -19.585 | 30.782 | 45.254 | 1.00 | 67.78  |
|    | ATOM | 697 | O   | PRO | A | 91 | -20.500 | 30.250 | 44.623 | 1.00 | 68.64  |
| 5  | ATOM | 698 | CB  | PRO | A | 91 | -19.843 | 33.213 | 44.738 | 1.00 | 59.70  |
|    | ATOM | 699 | CG  | PRO | A | 91 | -18.503 | 33.952 | 44.711 | 1.00 | 61.25  |
|    | ATOM | 700 | CD  | PRO | A | 91 | -17.731 | 33.539 | 45.961 | 1.00 | 54.16  |
|    | ATOM | 701 | N   | ILE | A | 92 | -18.413 | 30.177 | 45.416 | 1.00 | 64.82  |
|    | ATOM | 702 | CA  | ILE | A | 92 | -18.210 | 28.863 | 44.850 | 1.00 | 65.03  |
| 10 | ATOM | 703 | C   | ILE | A | 92 | -17.485 | 27.948 | 45.801 | 1.00 | 66.34  |
|    | ATOM | 704 | O   | ILE | A | 92 | -16.258 | 27.984 | 45.865 | 1.00 | 70.20  |
|    | ATOM | 705 | CB  | ILE | A | 92 | -17.433 | 28.927 | 43.547 | 1.00 | 69.56  |
|    | ATOM | 706 | CG1 | ILE | A | 92 | -18.298 | 29.495 | 42.430 | 1.00 | 70.02  |
|    | ATOM | 707 | CG2 | ILE | A | 92 | -16.975 | 27.517 | 43.171 | 1.00 | 71.86  |
|    | ATOM | 708 | CD1 | ILE | A | 92 | -17.528 | 29.672 | 41.121 | 1.00 | 80.63  |
| 15 | ATOM | 709 | N   | ALA | A | 93 | -18.219 | 27.115 | 46.534 | 1.00 | 54.40  |
|    | ATOM | 710 | CA  | ALA | A | 93 | -17.526 | 26.247 | 47.452 | 1.00 | 51.74  |
|    | ATOM | 711 | C   | ALA | A | 93 | -16.265 | 25.750 | 46.804 | 1.00 | 52.66  |
|    | ATOM | 712 | O   | ALA | A | 93 | -16.288 | 25.319 | 45.662 | 1.00 | 49.87  |
| 20 | ATOM | 713 | CB  | ALA | A | 93 | -18.367 | 25.101 | 47.968 | 1.00 | 52.76  |
|    | ATOM | 714 | N   | LEU | A | 94 | -15.162 | 25.861 | 47.544 | 1.00 | 48.18  |
|    | ATOM | 715 | CA  | LEU | A | 94 | -13.862 | 25.425 | 47.067 | 1.00 | 43.27  |
|    | ATOM | 716 | C   | LEU | A | 94 | -13.566 | 24.066 | 47.581 | 1.00 | 43.98  |
|    | ATOM | 717 | O   | LEU | A | 94 | -14.086 | 23.633 | 48.601 | 1.00 | 44.63  |
| 25 | ATOM | 718 | CB  | LEU | A | 94 | -12.713 | 26.344 | 47.509 | 1.00 | 41.05  |
|    | ATOM | 719 | CG  | LEU | A | 94 | -12.685 | 27.638 | 46.739 | 1.00 | 40.03  |
|    | ATOM | 720 | CD1 | LEU | A | 94 | -11.272 | 28.200 | 46.751 | 1.00 | 36.88  |
|    | ATOM | 721 | CD2 | LEU | A | 94 | -13.115 | 27.343 | 45.311 | 1.00 | 44.98  |
|    | ATOM | 722 | N   | SER | A | 95 | -12.706 | 23.406 | 46.875 | 1.00 | 43.26  |
|    | ATOM | 723 | CA  | SER | A | 95 | -12.321 | 22.074 | 47.256 | 1.00 | 43.76  |
| 30 | ATOM | 724 | C   | SER | A | 95 | -10.807 | 21.991 | 47.344 | 1.00 | 38.58  |
|    | ATOM | 725 | O   | SER | A | 95 | -10.087 | 22.944 | 46.975 | 1.00 | 36.78  |
|    | ATOM | 726 | CB  | SER | A | 95 | -12.902 | 21.092 | 46.256 | 1.00 | 51.55  |
|    | ATOM | 727 | OG  | SER | A | 95 | -14.299 | 21.305 | 46.156 | 1.00 | 62.74  |
|    | ATOM | 728 | N   | LYS | A | 96 | -10.321 | 20.863 | 47.830 | 1.00 | 31.10  |
| 35 | ATOM | 729 | CA  | LYS | A | 96 | -8.883  | 20.723 | 47.958 | 1.00 | 34.92  |
|    | ATOM | 730 | C   | LYS | A | 96 | -8.058  | 21.238 | 46.777 | 1.00 | 45.63  |
|    | ATOM | 731 | O   | LYS | A | 96 | -8.400  | 21.063 | 45.612 | 1.00 | 49.35  |
|    | ATOM | 732 | CB  | LYS | A | 96 | -8.401  | 19.366 | 48.451 | 1.00 | 38.53  |
|    | ATOM | 733 | CG  | LYS | A | 96 | -9.189  | 18.871 | 49.651 | 1.00 | 68.97  |
| 40 | ATOM | 734 | CD  | LYS | A | 96 | -8.691  | 17.549 | 50.221 | 1.00 | 80.86  |
|    | ATOM | 735 | CE  | LYS | A | 96 | -9.596  | 17.011 | 51.330 | 1.00 | 92.53  |
|    | ATOM | 736 | NZ  | LYS | A | 96 | -9.049  | 15.833 | 52.029 | 1.00 | 100.00 |
|    | ATOM | 737 | N   | ASN | A | 97 | -6.944  | 21.873 | 47.108 | 1.00 | 41.92  |
|    | ATOM | 738 | CA  | ASN | A | 97 | -6.009  | 22.403 | 46.139 | 1.00 | 40.91  |
| 45 | ATOM | 739 | C   | ASN | A | 97 | -6.606  | 23.348 | 45.088 | 1.00 | 42.64  |
|    | ATOM | 740 | O   | ASN | A | 97 | -5.963  | 23.681 | 44.068 | 1.00 | 38.69  |
|    | ATOM | 741 | CB  | ASN | A | 97 | -5.084  | 21.304 | 45.583 | 1.00 | 28.16  |
|    | ATOM | 742 | CG  | ASN | A | 97 | -4.327  | 20.568 | 46.677 | 1.00 | 52.21  |
|    | ATOM | 743 | OD1 | ASN | A | 97 | -3.089  | 20.627 | 46.744 | 1.00 | 55.30  |
| 50 | ATOM | 744 | ND2 | ASN | A | 97 | -5.060  | 19.858 | 47.533 | 1.00 | 53.87  |
|    | ATOM | 745 | N   | GLN | A | 98 | -7.833  | 23.791 | 45.382 | 1.00 | 36.59  |
|    | ATOM | 746 | CA  | GLN | A | 98 | -8.557  | 24.718 | 44.536 | 1.00 | 38.44  |
|    | ATOM | 747 | C   | GLN | A | 98 | -8.288  | 26.181 | 44.951 | 1.00 | 43.30  |
|    | ATOM | 748 | O   | GLN | A | 98 | -8.248  | 26.526 | 46.138 | 1.00 | 43.40  |
| 55 | ATOM | 749 | CB  | GLN | A | 98 | -10.064 | 24.395 | 44.575 | 1.00 | 42.26  |
|    | ATOM | 750 | CG  | GLN | A | 98 | -10.553 | 23.538 | 43.385 | 1.00 | 68.24  |
|    | ATOM | 751 | CD  | GLN | A | 98 | -12.008 | 23.778 | 43.010 | 1.00 | 95.57  |
|    | ATOM | 752 | OE1 | GLN | A | 98 | -12.890 | 22.935 | 43.278 | 1.00 | 86.92  |
|    | ATOM | 753 | NE2 | GLN | A | 98 | -12.271 | 24.935 | 42.393 | 1.00 | 95.48  |
| 60 | ATOM | 754 | N   | GLU | A | 99 | -8.089  | 27.062 | 43.973 | 1.00 | 39.70  |
|    | ATOM | 755 | CA  | GLU | A | 99 | -7.817  | 28.468 | 44.280 | 1.00 | 40.49  |
|    | ATOM | 756 | C   | GLU | A | 99 | -8.750  | 29.536 | 43.683 | 1.00 | 47.84  |
|    | ATOM | 757 | O   | GLU | A | 99 | -9.330  | 29.394 | 42.606 | 1.00 | 46.85  |
|    | ATOM | 758 | CB  | GLU | A | 99 | -6.361  | 28.866 | 43.951 | 1.00 | 40.24  |



|    |      |     |     |     |   |     |         |        |        |      |       |
|----|------|-----|-----|-----|---|-----|---------|--------|--------|------|-------|
|    | ATOM | 759 | CG  | GLU | A | 99  | -5.608  | 27.861 | 43.080 | 1.00 | 44.16 |
|    | ATOM | 760 | CD  | GLU | A | 99  | -4.120  | 28.119 | 42.990 | 1.00 | 65.64 |
|    | ATOM | 761 | OE1 | GLU | A | 99  | -3.636  | 29.062 | 42.376 | 1.00 | 73.95 |
| 5  | ATOM | 762 | OE2 | GLU | A | 99  | -3.395  | 27.210 | 43.614 | 1.00 | 55.99 |
|    | ATOM | 763 | N   | ILE | A | 100 | -8.848  | 30.643 | 44.418 | 1.00 | 43.55 |
|    | ATOM | 764 | CA  | ILE | A | 100 | -9.595  | 31.800 | 44.005 | 1.00 | 43.46 |
|    | ATOM | 765 | C   | ILE | A | 100 | -8.701  | 32.992 | 44.238 | 1.00 | 53.31 |
|    | ATOM | 766 | O   | ILE | A | 100 | -7.725  | 32.927 | 45.004 | 1.00 | 55.16 |
| 10 | ATOM | 767 | CB  | ILE | A | 100 | -10.881 | 32.068 | 44.773 | 1.00 | 46.65 |
|    | ATOM | 768 | CG1 | ILE | A | 100 | -10.762 | 31.640 | 46.227 | 1.00 | 50.76 |
|    | ATOM | 769 | CG2 | ILE | A | 100 | -12.111 | 31.486 | 44.106 | 1.00 | 46.76 |
|    | ATOM | 770 | CD1 | ILE | A | 100 | -9.959  | 32.620 | 47.087 | 1.00 | 64.36 |
|    | ATOM | 771 | N   | VAL | A | 101 | -9.060  | 34.076 | 43.580 | 1.00 | 48.20 |
| 15 | ATOM | 772 | CA  | VAL | A | 101 | -8.382  | 35.329 | 43.760 | 1.00 | 45.63 |
|    | ATOM | 773 | C   | VAL | A | 101 | -9.383  | 36.351 | 44.295 | 1.00 | 48.59 |
|    | ATOM | 774 | O   | VAL | A | 101 | -10.331 | 36.722 | 43.623 | 1.00 | 51.29 |
|    | ATOM | 775 | CB  | VAL | A | 101 | -7.461  | 35.793 | 42.633 | 1.00 | 45.06 |
|    | ATOM | 776 | CG1 | VAL | A | 101 | -7.693  | 35.000 | 41.378 | 1.00 | 43.25 |
| 20 | ATOM | 777 | CG2 | VAL | A | 101 | -7.609  | 37.289 | 42.395 | 1.00 | 45.02 |
|    | ATOM | 778 | N   | ILE | A | 102 | -9.182  | 36.738 | 45.546 | 1.00 | 41.15 |
|    | ATOM | 779 | CA  | ILE | A | 102 | -10.023 | 37.690 | 46.238 | 1.00 | 39.43 |
|    | ATOM | 780 | C   | ILE | A | 102 | -9.439  | 39.062 | 46.170 | 1.00 | 49.35 |
|    | ATOM | 781 | O   | ILE | A | 102 | -8.331  | 39.274 | 46.659 | 1.00 | 53.80 |
| 25 | ATOM | 782 | CB  | ILE | A | 102 | -10.097 | 37.319 | 47.694 | 1.00 | 39.19 |
|    | ATOM | 783 | CG1 | ILE | A | 102 | -10.180 | 35.800 | 47.809 | 1.00 | 35.28 |
|    | ATOM | 784 | CG2 | ILE | A | 102 | -11.300 | 37.992 | 48.341 | 1.00 | 35.25 |
|    | ATOM | 785 | CD1 | ILE | A | 102 | -10.962 | 35.392 | 49.044 | 1.00 | 47.09 |
|    | ATOM | 786 | N   | GLU | A | 103 | -10.192 | 39.984 | 45.572 | 1.00 | 43.20 |
| 30 | ATOM | 787 | CA  | GLU | A | 103 | -9.748  | 41.362 | 45.433 | 1.00 | 39.88 |
|    | ATOM | 788 | C   | GLU | A | 103 | -10.378 | 42.299 | 46.425 | 1.00 | 44.03 |
|    | ATOM | 789 | O   | GLU | A | 103 | -11.580 | 42.558 | 46.385 | 1.00 | 41.34 |
|    | ATOM | 790 | CB  | GLU | A | 103 | -9.950  | 41.930 | 44.047 | 1.00 | 39.11 |
|    | ATOM | 791 | CG  | GLU | A | 103 | -9.017  | 43.112 | 43.863 | 1.00 | 36.18 |
| 35 | ATOM | 792 | CD  | GLU | A | 103 | -9.150  | 43.666 | 42.485 | 1.00 | 61.93 |
|    | ATOM | 793 | OE1 | GLU | A | 103 | -10.157 | 44.234 | 42.100 | 1.00 | 69.89 |
|    | ATOM | 794 | OE2 | GLU | A | 103 | -8.087  | 43.457 | 41.744 | 1.00 | 76.18 |
|    | ATOM | 795 | N   | ILE | A | 104 | -9.534  | 42.797 | 47.322 | 1.00 | 42.69 |
|    | ATOM | 796 | CA  | ILE | A | 104 | -9.969  | 43.718 | 48.346 | 1.00 | 40.72 |
| 40 | ATOM | 797 | C   | ILE | A | 104 | -9.522  | 45.167 | 48.099 | 1.00 | 46.21 |
|    | ATOM | 798 | O   | ILE | A | 104 | -8.346  | 45.478 | 47.866 | 1.00 | 42.68 |
|    | ATOM | 799 | CB  | ILE | A | 104 | -9.578  | 43.283 | 49.754 | 1.00 | 41.75 |
|    | ATOM | 800 | CG1 | ILE | A | 104 | -10.006 | 41.855 | 50.032 | 1.00 | 39.85 |
|    | ATOM | 801 | CG2 | ILE | A | 104 | -10.225 | 44.222 | 50.768 | 1.00 | 41.53 |
| 45 | ATOM | 802 | CD1 | ILE | A | 104 | -8.839  | 40.995 | 50.485 | 1.00 | 34.17 |
|    | ATOM | 803 | N   | SER | A | 105 | -10.506 | 46.056 | 48.173 | 1.00 | 47.94 |
|    | ATOM | 804 | CA  | SER | A | 105 | -10.278 | 47.481 | 48.046 | 1.00 | 48.05 |
|    | ATOM | 805 | C   | SER | A | 105 | -10.184 | 47.977 | 49.482 | 1.00 | 42.39 |
|    | ATOM | 806 | O   | SER | A | 105 | -11.134 | 47.879 | 50.263 | 1.00 | 39.69 |
| 50 | ATOM | 807 | CB  | SER | A | 105 | -11.399 | 48.180 | 47.290 | 1.00 | 53.77 |
|    | ATOM | 808 | OG  | SER | A | 105 | -11.399 | 47.789 | 45.930 | 1.00 | 60.69 |
|    | ATOM | 809 | N   | PHE | A | 106 | -9.020  | 48.445 | 49.857 | 1.00 | 35.07 |
|    | ATOM | 810 | CA  | PHE | A | 106 | -8.844  | 48.890 | 51.223 | 1.00 | 34.98 |
|    | ATOM | 811 | C   | PHE | A | 106 | -8.177  | 50.238 | 51.262 | 1.00 | 39.26 |
| 55 | ATOM | 812 | O   | PHE | A | 106 | -7.607  | 50.730 | 50.265 | 1.00 | 34.24 |
|    | ATOM | 813 | CB  | PHE | A | 106 | -8.015  | 47.864 | 52.060 | 1.00 | 36.05 |
|    | ATOM | 814 | CG  | PHE | A | 106 | -6.581  | 47.815 | 51.556 | 1.00 | 37.24 |
|    | ATOM | 815 | CD1 | PHE | A | 106 | -6.251  | 47.073 | 50.422 | 1.00 | 39.71 |
|    | ATOM | 816 | CD2 | PHE | A | 106 | -5.579  | 48.579 | 52.161 | 1.00 | 36.44 |
| 60 | ATOM | 817 | CE1 | PHE | A | 106 | -4.950  | 47.086 | 49.920 | 1.00 | 41.48 |
|    | ATOM | 818 | CE2 | PHE | A | 106 | -4.273  | 48.609 | 51.672 | 1.00 | 38.19 |
|    | ATOM | 819 | CZ  | PHE | A | 106 | -3.961  | 47.856 | 50.540 | 1.00 | 37.91 |
|    | ATOM | 820 | N   | GLU | A | 107 | -8.284  | 50.794 | 52.453 | 1.00 | 40.64 |
|    | ATOM | 821 | CA  | GLU | A | 107 | -7.711  | 52.064 | 52.848 | 1.00 | 43.81 |
|    | ATOM | 822 | C   | GLU | A | 107 | -7.206  | 51.869 | 54.284 | 1.00 | 43.82 |



|    |      |     |     |     |   |     |         |        |        |      |        |
|----|------|-----|-----|-----|---|-----|---------|--------|--------|------|--------|
|    | ATOM | 823 | O   | GLU | A | 107 | -7.933  | 51.303 | 55.121 | 1.00 | 38.38  |
|    | ATOM | 824 | CB  | GLU | A | 107 | -8.737  | 53.234 | 52.753 | 1.00 | 46.93  |
|    | ATOM | 825 | CG  | GLU | A | 107 | -8.107  | 54.637 | 52.467 | 1.00 | 67.21  |
| 5  | ATOM | 826 | CD  | GLU | A | 107 | -9.086  | 55.715 | 52.042 | 1.00 | 100.00 |
|    | ATOM | 827 | OE1 | GLU | A | 107 | -10.208 | 55.504 | 51.599 | 1.00 | 100.00 |
|    | ATOM | 828 | OE2 | GLU | A | 107 | -8.631  | 56.938 | 52.221 | 1.00 | 93.72  |
|    | ATOM | 829 | N   | THR | A | 108 | -5.963  | 52.294 | 54.551 | 1.00 | 39.12  |
|    | ATOM | 830 | CA  | THR | A | 108 | -5.345  | 52.175 | 55.873 | 1.00 | 39.69  |
| 10 | ATOM | 831 | C   | THR | A | 108 | -5.564  | 53.427 | 56.724 | 1.00 | 49.82  |
|    | ATOM | 832 | O   | THR | A | 108 | -5.565  | 54.552 | 56.177 | 1.00 | 50.94  |
|    | ATOM | 833 | CB  | THR | A | 108 | -3.810  | 52.095 | 55.722 | 1.00 | 40.40  |
|    | ATOM | 834 | OG1 | THR | A | 108 | -3.360  | 53.226 | 54.981 | 1.00 | 32.22  |
|    | ATOM | 835 | CG2 | THR | A | 108 | -3.371  | 50.802 | 55.042 | 1.00 | 46.43  |
| 15 | ATOM | 836 | N   | SER | A | 109 | -5.698  | 53.217 | 58.065 | 1.00 | 42.02  |
|    | ATOM | 837 | CA  | SER | A | 109 | -5.848  | 54.294 | 59.038 | 1.00 | 38.13  |
|    | ATOM | 838 | C   | SER | A | 109 | -4.555  | 55.101 | 59.082 | 1.00 | 38.47  |
|    | ATOM | 839 | O   | SER | A | 109 | -3.460  | 54.583 | 58.921 | 1.00 | 33.60  |
|    | ATOM | 840 | CB  | SER | A | 109 | -6.166  | 53.759 | 60.437 | 1.00 | 41.44  |
| 20 | ATOM | 841 | OG  | SER | A | 109 | -6.205  | 54.812 | 61.404 | 1.00 | 47.63  |
|    | ATOM | 842 | N   | PRO | A | 110 | -4.655  | 56.392 | 59.308 | 1.00 | 41.64  |
|    | ATOM | 843 | CA  | PRO | A | 110 | -3.419  | 57.116 | 59.393 | 1.00 | 40.75  |
|    | ATOM | 844 | C   | PRO | A | 110 | -2.803  | 56.749 | 60.725 | 1.00 | 41.47  |
|    | ATOM | 845 | O   | PRO | A | 110 | -1.676  | 57.080 | 61.009 | 1.00 | 42.30  |
| 25 | ATOM | 846 | CB  | PRO | A | 110 | -3.721  | 58.605 | 59.298 | 1.00 | 42.09  |
|    | ATOM | 847 | CG  | PRO | A | 110 | -5.224  | 58.719 | 59.132 | 1.00 | 48.77  |
|    | ATOM | 848 | CD  | PRO | A | 110 | -5.811  | 57.318 | 59.269 | 1.00 | 44.58  |
|    | ATOM | 849 | N   | LYS | A | 111 | -3.578  | 56.017 | 61.518 | 1.00 | 36.35  |
|    | ATOM | 850 | CA  | LYS | A | 111 | -3.167  | 55.535 | 62.819 | 1.00 | 36.74  |
| 30 | ATOM | 851 | C   | LYS | A | 111 | -2.669  | 54.083 | 62.720 | 1.00 | 40.19  |
|    | ATOM | 852 | O   | LYS | A | 111 | -2.733  | 53.319 | 63.678 | 1.00 | 40.53  |
|    | ATOM | 853 | CB  | LYS | A | 111 | -4.341  | 55.606 | 63.807 | 1.00 | 41.91  |
|    | ATOM | 854 | CG  | LYS | A | 111 | -4.362  | 56.838 | 64.708 | 1.00 | 71.21  |
|    | ATOM | 855 | CD  | LYS | A | 111 | -5.421  | 57.854 | 64.309 | 1.00 | 97.95  |
| 35 | ATOM | 856 | CE  | LYS | A | 111 | -6.839  | 57.394 | 64.611 | 1.00 | 100.00 |
|    | ATOM | 857 | NZ  | LYS | A | 111 | -7.853  | 58.120 | 63.819 | 1.00 | 100.00 |
|    | ATOM | 858 | N   | SER | A | 112 | -2.184  | 53.670 | 61.550 | 1.00 | 36.84  |
|    | ATOM | 859 | CA  | SER | A | 112 | -1.714  | 52.296 | 61.358 | 1.00 | 34.35  |
|    | ATOM | 860 | C   | SER | A | 112 | -0.518  | 51.917 | 62.225 | 1.00 | 35.57  |
| 40 | ATOM | 861 | O   | SER | A | 112 | 0.533   | 52.548 | 62.166 | 1.00 | 32.49  |
|    | ATOM | 862 | CB  | SER | A | 112 | -1.449  | 51.995 | 59.883 | 1.00 | 35.16  |
|    | ATOM | 863 | OG  | SER | A | 112 | -0.682  | 50.814 | 59.762 | 1.00 | 31.94  |
|    | ATOM | 864 | N   | SER | A | 113 | -0.666  | 50.872 | 63.033 | 1.00 | 31.84  |
|    | ATOM | 865 | CA  | SER | A | 113 | 0.445   | 50.460 | 63.866 | 1.00 | 29.27  |
| 45 | ATOM | 866 | C   | SER | A | 113 | 1.601   | 49.927 | 63.040 | 1.00 | 33.37  |
|    | ATOM | 867 | O   | SER | A | 113 | 2.715   | 49.792 | 63.497 | 1.00 | 32.95  |
|    | ATOM | 868 | CB  | SER | A | 113 | 0.052   | 49.498 | 64.945 | 1.00 | 29.45  |
|    | ATOM | 869 | OG  | SER | A | 113 | 0.045   | 48.169 | 64.462 | 1.00 | 34.27  |
|    | ATOM | 870 | N   | ALA | A | 114 | 1.357   | 49.628 | 61.797 | 1.00 | 33.69  |
| 50 | ATOM | 871 | CA  | ALA | A | 114 | 2.437   | 49.134 | 60.981 | 1.00 | 34.05  |
|    | ATOM | 872 | C   | ALA | A | 114 | 3.239   | 50.287 | 60.388 | 1.00 | 37.83  |
|    | ATOM | 873 | O   | ALA | A | 114 | 4.411   | 50.149 | 60.033 | 1.00 | 37.72  |
|    | ATOM | 874 | CB  | ALA | A | 114 | 1.845   | 48.292 | 59.852 | 1.00 | 34.51  |
|    | ATOM | 875 | N   | LEU | A | 115 | 2.580   | 51.432 | 60.259 | 1.00 | 32.19  |
| 55 | ATOM | 876 | CA  | LEU | A | 115 | 3.201   | 52.595 | 59.662 | 1.00 | 30.48  |
|    | ATOM | 877 | C   | LEU | A | 115 | 3.509   | 53.745 | 60.565 | 1.00 | 35.32  |
|    | ATOM | 878 | O   | LEU | A | 115 | 2.902   | 54.012 | 61.604 | 1.00 | 35.25  |
|    | ATOM | 879 | CB  | LEU | A | 115 | 2.358   | 53.156 | 58.507 | 1.00 | 30.53  |
|    | ATOM | 880 | CG  | LEU | A | 115 | 1.787   | 52.064 | 57.602 | 1.00 | 35.51  |
| 60 | ATOM | 881 | CD1 | LEU | A | 115 | 0.812   | 52.710 | 56.637 | 1.00 | 35.12  |
|    | ATOM | 882 | CD2 | LEU | A | 115 | 2.903   | 51.387 | 56.821 | 1.00 | 33.88  |
|    | ATOM | 883 | N   | GLN | A | 116 | 4.490   | 54.457 | 60.096 | 1.00 | 34.00  |
|    | ATOM | 884 | CA  | GLN | A | 116 | 4.926   | 55.656 | 60.737 | 1.00 | 32.52  |
|    | ATOM | 885 | C   | GLN | A | 116 | 5.066   | 56.689 | 59.645 | 1.00 | 31.34  |
|    | ATOM | 886 | O   | GLN | A | 116 | 5.880   | 56.552 | 58.729 | 1.00 | 28.29  |



|    |      |     |     |     |   |     |        |        |        |      |        |
|----|------|-----|-----|-----|---|-----|--------|--------|--------|------|--------|
|    | ATOM | 887 | CB  | GLN | A | 116 | 6.232  | 55.540 | 61.496 | 1.00 | 32.66  |
|    | ATOM | 888 | CG  | GLN | A | 116 | 6.419  | 56.813 | 62.322 | 1.00 | 41.25  |
|    | ATOM | 889 | CD  | GLN | A | 116 | 7.777  | 56.897 | 62.952 | 1.00 | 50.08  |
| 5  | ATOM | 890 | OE1 | GLN | A | 116 | 8.515  | 55.905 | 63.017 | 1.00 | 55.36  |
|    | ATOM | 891 | NE2 | GLN | A | 116 | 8.090  | 58.081 | 63.438 | 1.00 | 38.23  |
|    | ATOM | 892 | N   | TRP | A | 117 | 4.210  | 57.680 | 59.748 | 1.00 | 26.66  |
|    | ATOM | 893 | CA  | TRP | A | 117 | 4.148  | 58.785 | 58.827 | 1.00 | 26.04  |
|    | ATOM | 894 | C   | TRP | A | 117 | 4.912  | 59.978 | 59.375 | 1.00 | 34.56  |
| 10 | ATOM | 895 | O   | TRP | A | 117 | 4.467  | 60.589 | 60.364 | 1.00 | 36.83  |
|    | ATOM | 896 | CB  | TRP | A | 117 | 2.669  | 59.188 | 58.630 | 1.00 | 23.15  |
|    | ATOM | 897 | CG  | TRP | A | 117 | 1.826  | 58.209 | 57.863 | 1.00 | 23.02  |
|    | ATOM | 898 | CD1 | TRP | A | 117 | 1.052  | 57.224 | 58.397 | 1.00 | 26.39  |
|    | ATOM | 899 | CD2 | TRP | A | 117 | 1.640  | 58.135 | 56.433 | 1.00 | 21.06  |
| 15 | ATOM | 900 | NE1 | TRP | A | 117 | 0.395  | 56.534 | 57.393 | 1.00 | 26.40  |
|    | ATOM | 901 | CE2 | TRP | A | 117 | 0.735  | 57.087 | 56.184 | 1.00 | 27.99  |
|    | ATOM | 902 | CE3 | TRP | A | 117 | 2.121  | 58.872 | 55.361 | 1.00 | 20.95  |
|    | ATOM | 903 | CZ2 | TRP | A | 117 | 0.352  | 56.753 | 54.886 | 1.00 | 28.21  |
|    | ATOM | 904 | CZ3 | TRP | A | 117 | 1.750  | 58.560 | 54.079 | 1.00 | 22.43  |
| 20 | ATOM | 905 | CH2 | TRP | A | 117 | 0.872  | 57.512 | 53.847 | 1.00 | 24.28  |
|    | ATOM | 906 | N   | LEU | A | 118 | 6.043  | 60.340 | 58.756 | 1.00 | 31.44  |
|    | ATOM | 907 | CA  | LEU | A | 118 | 6.745  | 61.506 | 59.276 | 1.00 | 36.67  |
|    | ATOM | 908 | C   | LEU | A | 118 | 6.584  | 62.774 | 58.432 | 1.00 | 46.93  |
|    | ATOM | 909 | O   | LEU | A | 118 | 6.434  | 62.705 | 57.210 | 1.00 | 51.17  |
| 25 | ATOM | 910 | CB  | LEU | A | 118 | 8.250  | 61.327 | 59.577 | 1.00 | 38.83  |
|    | ATOM | 911 | CG  | LEU | A | 118 | 8.881  | 59.939 | 59.398 | 1.00 | 44.33  |
|    | ATOM | 912 | CD1 | LEU | A | 118 | 10.392 | 60.065 | 59.569 | 1.00 | 42.12  |
|    | ATOM | 913 | CD2 | LEU | A | 118 | 8.351  | 58.950 | 60.426 | 1.00 | 49.99  |
|    | ATOM | 914 | N   | THR | A | 119 | 6.524  | 63.939 | 59.109 | 1.00 | 41.34  |
| 30 | ATOM | 915 | CA  | THR | A | 119 | 6.449  | 65.260 | 58.468 | 1.00 | 38.89  |
|    | ATOM | 916 | C   | THR | A | 119 | 7.847  | 65.633 | 58.034 | 1.00 | 40.14  |
|    | ATOM | 917 | O   | THR | A | 119 | 8.841  | 65.165 | 58.605 | 1.00 | 44.03  |
|    | ATOM | 918 | CB  | THR | A | 119 | 5.932  | 66.300 | 59.467 | 1.00 | 42.63  |
|    | ATOM | 919 | OG1 | THR | A | 119 | 6.994  | 66.605 | 60.362 | 1.00 | 50.01  |
| 35 | ATOM | 920 | CG2 | THR | A | 119 | 4.769  | 65.668 | 60.224 | 1.00 | 36.78  |
|    | ATOM | 921 | N   | PRO | A | 120 | 7.963  | 66.440 | 57.020 | 1.00 | 33.41  |
|    | ATOM | 922 | CA  | PRO | A | 120 | 9.275  | 66.781 | 56.517 | 1.00 | 33.18  |
|    | ATOM | 923 | C   | PRO | A | 120 | 10.260 | 67.209 | 57.599 | 1.00 | 38.27  |
|    | ATOM | 924 | O   | PRO | A | 120 | 11.433 | 66.829 | 57.566 | 1.00 | 34.42  |
| 40 | ATOM | 925 | CB  | PRO | A | 120 | 9.068  | 67.840 | 55.416 | 1.00 | 33.54  |
|    | ATOM | 926 | CG  | PRO | A | 120 | 7.582  | 67.823 | 55.097 | 1.00 | 34.86  |
|    | ATOM | 927 | CD  | PRO | A | 120 | 6.891  | 67.180 | 56.300 | 1.00 | 30.86  |
|    | ATOM | 928 | N   | GLU | A | 121 | 9.751  | 67.982 | 58.563 | 1.00 | 38.03  |
|    | ATOM | 929 | CA  | GLU | A | 121 | 10.534 | 68.474 | 59.681 | 1.00 | 41.03  |
| 45 | ATOM | 930 | C   | GLU | A | 121 | 11.212 | 67.361 | 60.411 | 1.00 | 50.88  |
|    | ATOM | 931 | O   | GLU | A | 121 | 12.279 | 67.548 | 60.977 | 1.00 | 54.97  |
|    | ATOM | 932 | CB  | GLU | A | 121 | 9.742  | 69.325 | 60.699 | 1.00 | 43.28  |
|    | ATOM | 933 | CG  | GLU | A | 121 | 8.220  | 69.071 | 60.702 | 1.00 | 64.72  |
|    | ATOM | 934 | CD  | GLU | A | 121 | 7.398  | 70.118 | 59.988 | 1.00 | 86.07  |
| 50 | ATOM | 935 | OE1 | GLU | A | 121 | 7.007  | 71.131 | 60.538 | 1.00 | 100.00 |
|    | ATOM | 936 | OE2 | GLU | A | 121 | 7.108  | 69.803 | 58.739 | 1.00 | 59.72  |
|    | ATOM | 937 | N   | GLN | A | 122 | 10.569 | 66.202 | 60.394 | 1.00 | 44.09  |
|    | ATOM | 938 | CA  | GLN | A | 122 | 11.083 | 65.019 | 61.041 | 1.00 | 40.20  |
|    | ATOM | 939 | C   | GLN | A | 122 | 12.170 | 64.373 | 60.232 | 1.00 | 47.73  |
| 55 | ATOM | 940 | O   | GLN | A | 122 | 12.711 | 63.343 | 60.643 | 1.00 | 53.29  |
|    | ATOM | 941 | CB  | GLN | A | 122 | 9.965  | 63.992 | 61.224 | 1.00 | 39.31  |
|    | ATOM | 942 | CG  | GLN | A | 122 | 9.057  | 64.441 | 62.361 | 1.00 | 30.23  |
|    | ATOM | 943 | CD  | GLN | A | 122 | 7.756  | 63.691 | 62.438 | 1.00 | 38.25  |
|    | ATOM | 944 | OE1 | GLN | A | 122 | 6.899  | 63.804 | 61.548 | 1.00 | 53.34  |
| 60 | ATOM | 945 | NE2 | GLN | A | 122 | 7.592  | 62.938 | 63.521 | 1.00 | 18.98  |
|    | ATOM | 946 | N   | THR | A | 123 | 12.486 | 64.942 | 59.074 | 1.00 | 38.99  |
|    | ATOM | 947 | CA  | THR | A | 123 | 13.490 | 64.319 | 58.229 | 1.00 | 36.00  |
|    | ATOM | 948 | C   | THR | A | 123 | 14.755 | 65.034 | 58.264 | 1.00 | 35.30  |
|    | ATOM | 949 | O   | THR | A | 123 | 14.842 | 66.074 | 58.875 | 1.00 | 34.95  |
|    | ATOM | 950 | CB  | THR | A | 123 | 13.067 | 64.145 | 56.759 | 1.00 | 38.25  |



|    |      |      |     |     |   |     |        |        |        |      |        |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
|    | ATOM | 951  | OG1 | THR | A | 123 | 13.144 | 65.374 | 56.046 | 1.00 | 43.75  |
|    | ATOM | 952  | CG2 | THR | A | 123 | 11.643 | 63.616 | 56.725 | 1.00 | 40.72  |
|    | ATOM | 953  | N   | SER | A | 124 | 15.699 | 64.447 | 57.557 | 1.00 | 32.18  |
| 5  | ATOM | 954  | CA  | SER | A | 124 | 17.025 | 64.996 | 57.442 | 1.00 | 33.71  |
|    | ATOM | 955  | C   | SER | A | 124 | 17.007 | 66.216 | 56.553 | 1.00 | 39.04  |
|    | ATOM | 956  | O   | SER | A | 124 | 17.537 | 67.268 | 56.883 | 1.00 | 39.07  |
|    | ATOM | 957  | CB  | SER | A | 124 | 18.023 | 63.992 | 56.859 | 1.00 | 37.73  |
|    | ATOM | 958  | OG  | SER | A | 124 | 18.359 | 62.978 | 57.796 | 1.00 | 36.28  |
| 10 | ATOM | 959  | N   | GLY | A | 125 | 16.389 | 66.025 | 55.414 | 1.00 | 38.59  |
|    | ATOM | 960  | CA  | GLY | A | 125 | 16.280 | 67.034 | 54.396 | 1.00 | 39.90  |
|    | ATOM | 961  | C   | GLY | A | 125 | 15.290 | 68.094 | 54.749 | 1.00 | 46.83  |
|    | ATOM | 962  | O   | GLY | A | 125 | 15.347 | 69.171 | 54.172 | 1.00 | 49.78  |
|    | ATOM | 963  | N   | LYS | A | 126 | 14.391 | 67.788 | 55.678 | 1.00 | 41.09  |
| 15 | ATOM | 964  | CA  | LYS | A | 126 | 13.396 | 68.761 | 56.126 | 1.00 | 41.26  |
|    | ATOM | 965  | C   | LYS | A | 126 | 12.498 | 69.307 | 55.020 | 1.00 | 47.42  |
|    | ATOM | 966  | O   | LYS | A | 126 | 11.617 | 70.141 | 55.279 | 1.00 | 48.94  |
|    | ATOM | 967  | CB  | LYS | A | 126 | 14.024 | 69.936 | 56.894 | 1.00 | 41.98  |
|    | ATOM | 968  | CG  | LYS | A | 126 | 15.094 | 69.555 | 57.913 | 1.00 | 45.84  |
| 20 | ATOM | 969  | CD  | LYS | A | 126 | 14.535 | 68.838 | 59.135 | 1.00 | 58.74  |
|    | ATOM | 970  | CE  | LYS | A | 126 | 15.612 | 68.500 | 60.151 | 1.00 | 72.12  |
|    | ATOM | 971  | NZ  | LYS | A | 126 | 15.395 | 67.218 | 60.839 | 1.00 | 88.38  |
|    | ATOM | 972  | N   | GLU | A | 127 | 12.722 | 68.858 | 53.792 | 1.00 | 41.82  |
|    | ATOM | 973  | CA  | GLU | A | 127 | 11.921 | 69.344 | 52.708 | 1.00 | 41.98  |
| 25 | ATOM | 974  | C   | GLU | A | 127 | 10.899 | 68.334 | 52.239 | 1.00 | 45.14  |
|    | ATOM | 975  | O   | GLU | A | 127 | 9.994  | 68.683 | 51.496 | 1.00 | 46.95  |
|    | ATOM | 976  | CB  | GLU | A | 127 | 12.727 | 70.015 | 51.543 | 1.00 | 44.39  |
|    | ATOM | 977  | CG  | GLU | A | 127 | 13.198 | 71.499 | 51.820 | 1.00 | 57.99  |
|    | ATOM | 978  | CD  | GLU | A | 127 | 12.331 | 72.659 | 51.301 | 1.00 | 100.00 |
|    | ATOM | 979  | OE1 | GLU | A | 127 | 11.652 | 72.611 | 50.286 | 1.00 | 100.00 |
| 30 | ATOM | 980  | OE2 | GLU | A | 127 | 12.387 | 73.758 | 52.054 | 1.00 | 100.00 |
|    | ATOM | 981  | N   | HIS | A | 128 | 11.027 | 67.077 | 52.653 | 1.00 | 39.18  |
|    | ATOM | 982  | CA  | HIS | A | 128 | 10.068 | 66.072 | 52.210 | 1.00 | 39.43  |
|    | ATOM | 983  | C   | HIS | A | 128 | 9.636  | 65.148 | 53.316 | 1.00 | 42.09  |
| 35 | ATOM | 984  | O   | HIS | A | 128 | 10.366 | 64.955 | 54.281 | 1.00 | 45.34  |
|    | ATOM | 985  | CB  | HIS | A | 128 | 10.628 | 65.194 | 51.097 | 1.00 | 42.16  |
|    | ATOM | 986  | CG  | HIS | A | 128 | 10.947 | 65.936 | 49.854 | 1.00 | 47.24  |
|    | ATOM | 987  | ND1 | HIS | A | 128 | 9.943  | 66.423 | 49.029 | 1.00 | 49.12  |
|    | ATOM | 988  | CD2 | HIS | A | 128 | 12.159 | 66.262 | 49.322 | 1.00 | 51.13  |
| 40 | ATOM | 989  | CE1 | HIS | A | 128 | 10.559 | 67.031 | 48.026 | 1.00 | 49.97  |
|    | ATOM | 990  | NE2 | HIS | A | 128 | 11.888 | 66.953 | 48.166 | 1.00 | 50.87  |
|    | ATOM | 991  | N   | PRO | A | 129 | 8.447  | 64.572 | 53.171 | 1.00 | 32.55  |
|    | ATOM | 992  | CA  | PRO | A | 129 | 7.968  | 63.650 | 54.163 | 1.00 | 31.15  |
|    | ATOM | 993  | C   | PRO | A | 129 | 8.636  | 62.328 | 53.900 | 1.00 | 34.90  |
| 45 | ATOM | 994  | O   | PRO | A | 129 | 9.481  | 62.214 | 53.021 | 1.00 | 35.46  |
|    | ATOM | 995  | CB  | PRO | A | 129 | 6.466  | 63.490 | 53.986 | 1.00 | 31.94  |
|    | ATOM | 996  | CG  | PRO | A | 129 | 6.133  | 64.104 | 52.649 | 1.00 | 36.83  |
|    | ATOM | 997  | CD  | PRO | A | 129 | 7.384  | 64.850 | 52.185 | 1.00 | 32.71  |
|    | ATOM | 998  | N   | TYR | A | 130 | 8.248  | 61.342 | 54.659 | 1.00 | 29.47  |
|    | ATOM | 999  | CA  | TYR | A | 130 | 8.826  | 60.025 | 54.548 | 1.00 | 29.35  |
| 50 | ATOM | 1000 | C   | TYR | A | 130 | 7.856  | 59.046 | 55.156 | 1.00 | 31.83  |
|    | ATOM | 1001 | O   | TYR | A | 130 | 7.138  | 59.375 | 56.093 | 1.00 | 29.84  |
|    | ATOM | 1002 | CB  | TYR | A | 130 | 10.098 | 60.029 | 55.433 | 1.00 | 30.54  |
|    | ATOM | 1003 | CG  | TYR | A | 130 | 11.083 | 58.886 | 55.285 | 1.00 | 29.76  |
| 55 | ATOM | 1004 | CD1 | TYR | A | 130 | 10.845 | 57.630 | 55.845 | 1.00 | 26.16  |
|    | ATOM | 1005 | CD2 | TYR | A | 130 | 12.290 | 59.110 | 54.619 | 1.00 | 30.28  |
|    | ATOM | 1006 | CE1 | TYR | A | 130 | 11.795 | 56.621 | 55.721 | 1.00 | 17.87  |
|    | ATOM | 1007 | CE2 | TYR | A | 130 | 13.253 | 58.114 | 54.479 | 1.00 | 27.75  |
|    | ATOM | 1008 | CZ  | TYR | A | 130 | 12.983 | 56.866 | 55.031 | 1.00 | 25.76  |
| 60 | ATOM | 1009 | OH  | TYR | A | 130 | 13.899 | 55.864 | 54.894 | 1.00 | 40.52  |
|    | ATOM | 1010 | N   | LEU | A | 131 | 7.832  | 57.842 | 54.647 | 1.00 | 31.12  |
|    | ATOM | 1011 | CA  | LEU | A | 131 | 6.994  | 56.868 | 55.303 | 1.00 | 30.43  |
|    | ATOM | 1012 | C   | LEU | A | 131 | 7.691  | 55.568 | 55.289 | 1.00 | 33.91  |
|    | ATOM | 1013 | O   | LEU | A | 131 | 8.398  | 55.257 | 54.397 | 1.00 | 33.68  |
|    | ATOM | 1014 | CB  | LEU | A | 131 | 5.679  | 56.761 | 54.530 | 1.00 | 26.16  |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
|    | ATOM | 1015 | CG  | LEU | A | 131 | 5.065  | 55.367 | 54.600 | 1.00 | 21.68 |
|    | ATOM | 1016 | CD1 | LEU | A | 131 | 4.163  | 55.206 | 55.797 | 1.00 | 17.56 |
|    | ATOM | 1017 | CD2 | LEU | A | 131 | 4.222  | 55.008 | 53.380 | 1.00 | 13.86 |
| 5  | ATOM | 1018 | N   | PHE | A | 132 | 7.533  | 54.828 | 56.348 | 1.00 | 29.24 |
|    | ATOM | 1019 | CA  | PHE | A | 132 | 8.129  | 53.527 | 56.323 | 1.00 | 33.44 |
|    | ATOM | 1020 | C   | PHE | A | 132 | 7.299  | 52.519 | 57.157 | 1.00 | 41.08 |
|    | ATOM | 1021 | O   | PHE | A | 132 | 6.344  | 52.889 | 57.837 | 1.00 | 46.05 |
|    | ATOM | 1022 | CB  | PHE | A | 132 | 9.621  | 53.670 | 56.791 | 1.00 | 36.40 |
| 10 | ATOM | 1023 | CG  | PHE | A | 132 | 9.763  | 53.895 | 58.256 | 1.00 | 38.11 |
|    | ATOM | 1024 | CD1 | PHE | A | 132 | 9.601  | 52.821 | 59.053 | 1.00 | 37.18 |
|    | ATOM | 1025 | CD2 | PHE | A | 132 | 10.123 | 55.158 | 58.803 | 1.00 | 43.89 |
|    | ATOM | 1026 | CE1 | PHE | A | 132 | 9.771  | 52.936 | 60.422 | 1.00 | 41.04 |
|    | ATOM | 1027 | CE2 | PHE | A | 132 | 10.289 | 55.258 | 60.174 | 1.00 | 47.72 |
|    | ATOM | 1028 | CZ  | PHE | A | 132 | 10.131 | 54.143 | 60.986 | 1.00 | 44.34 |
| 15 | ATOM | 1029 | N   | SER | A | 133 | 7.612  | 51.221 | 57.002 | 1.00 | 33.47 |
|    | ATOM | 1030 | CA  | SER | A | 133 | 6.744  | 50.228 | 57.629 | 1.00 | 29.86 |
|    | ATOM | 1031 | C   | SER | A | 133 | 7.499  | 49.221 | 58.504 | 1.00 | 31.53 |
|    | ATOM | 1032 | O   | SER | A | 133 | 8.724  | 49.146 | 58.531 | 1.00 | 33.16 |
| 20 | ATOM | 1033 | CB  | SER | A | 133 | 5.942  | 49.481 | 56.535 | 1.00 | 33.19 |
|    | ATOM | 1034 | OG  | SER | A | 133 | 6.757  | 48.480 | 55.926 | 1.00 | 50.66 |
|    | ATOM | 1035 | N   | GLN | A | 134 | 6.703  | 48.466 | 59.294 | 1.00 | 24.61 |
|    | ATOM | 1036 | CA  | GLN | A | 134 | 7.283  | 47.422 | 60.134 | 1.00 | 22.55 |
|    | ATOM | 1037 | C   | GLN | A | 134 | 6.268  | 46.321 | 60.398 | 1.00 | 27.28 |
| 25 | ATOM | 1038 | O   | GLN | A | 134 | 5.161  | 46.566 | 60.809 | 1.00 | 25.09 |
|    | ATOM | 1039 | CB  | GLN | A | 134 | 7.711  | 48.041 | 61.464 | 1.00 | 23.29 |
|    | ATOM | 1040 | CG  | GLN | A | 134 | 8.218  | 46.987 | 62.454 | 1.00 | 25.96 |
|    | ATOM | 1041 | CD  | GLN | A | 134 | 9.423  | 46.290 | 61.872 | 1.00 | 25.65 |
|    | ATOM | 1042 | OE1 | GLN | A | 134 | 10.296 | 46.876 | 61.263 | 1.00 | 26.36 |
| 30 | ATOM | 1043 | NE2 | GLN | A | 134 | 9.445  | 44.965 | 62.095 | 1.00 | 21.75 |
|    | ATOM | 1044 | N   | CYS | A | 135 | 6.435  | 45.124 | 59.820 | 1.00 | 29.60 |
|    | ATOM | 1045 | CA  | CYS | A | 135 | 5.291  | 44.220 | 59.755 | 1.00 | 32.30 |
|    | ATOM | 1046 | C   | CYS | A | 135 | 5.442  | 43.006 | 60.662 | 1.00 | 39.58 |
|    | ATOM | 1047 | O   | CYS | A | 135 | 4.597  | 42.144 | 60.739 | 1.00 | 40.94 |
| 35 | ATOM | 1048 | CB  | CYS | A | 135 | 5.098  | 43.794 | 58.320 | 1.00 | 35.40 |
|    | ATOM | 1049 | SG  | CYS | A | 135 | 3.976  | 44.922 | 57.445 | 1.00 | 41.22 |
|    | ATOM | 1050 | N   | GLN | A | 136 | 6.582  | 42.949 | 61.345 | 1.00 | 37.37 |
|    | ATOM | 1051 | CA  | GLN | A | 136 | 6.715  | 41.982 | 62.417 | 1.00 | 35.71 |
|    | ATOM | 1052 | C   | GLN | A | 136 | 6.589  | 42.645 | 63.797 | 1.00 | 31.90 |
| 40 | ATOM | 1053 | O   | GLN | A | 136 | 6.878  | 43.803 | 63.981 | 1.00 | 30.54 |
|    | ATOM | 1054 | CB  | GLN | A | 136 | 8.077  | 41.311 | 62.295 | 1.00 | 37.24 |
|    | ATOM | 1055 | CG  | GLN | A | 136 | 8.076  | 39.878 | 62.847 | 1.00 | 29.70 |
|    | ATOM | 1056 | CD  | GLN | A | 136 | 9.483  | 39.511 | 63.235 | 1.00 | 36.48 |
|    | ATOM | 1057 | OE1 | GLN | A | 136 | 10.366 | 40.328 | 63.356 | 1.00 | 24.49 |
| 45 | ATOM | 1058 | NE2 | GLN | A | 136 | 9.665  | 38.201 | 63.443 | 1.00 | 22.19 |
|    | ATOM | 1059 | N   | ALA | A | 137 | 5.850  | 41.899 | 64.648 | 1.00 | 28.56 |
|    | ATOM | 1060 | CA  | ALA | A | 137 | 5.235  | 40.581 | 64.351 | 1.00 | 28.89 |
|    | ATOM | 1061 | C   | ALA | A | 137 | 3.860  | 40.503 | 63.630 | 1.00 | 31.83 |
|    | ATOM | 1062 | O   | ALA | A | 137 | 3.679  | 39.688 | 62.738 | 1.00 | 29.67 |
| 50 | ATOM | 1063 | CB  | ALA | A | 137 | 5.091  | 39.742 | 65.625 | 1.00 | 28.91 |
|    | ATOM | 1064 | N   | ILE | A | 138 | 2.863  | 41.285 | 64.070 | 1.00 | 27.07 |
|    | ATOM | 1065 | CA  | ILE | A | 138 | 1.553  | 41.176 | 63.445 | 1.00 | 23.90 |
|    | ATOM | 1066 | C   | ILE | A | 138 | 0.960  | 42.492 | 63.053 | 1.00 | 28.69 |
|    | ATOM | 1067 | O   | ILE | A | 138 | -0.144 | 42.822 | 63.426 | 1.00 | 31.92 |
| 55 | ATOM | 1068 | CB  | ILE | A | 138 | 0.641  | 40.357 | 64.339 | 1.00 | 25.41 |
|    | ATOM | 1069 | CG1 | ILE | A | 138 | 0.871  | 40.811 | 65.801 | 1.00 | 27.32 |
|    | ATOM | 1070 | CG2 | ILE | A | 138 | 1.162  | 38.938 | 64.191 | 1.00 | 16.34 |
|    | ATOM | 1071 | CD1 | ILE | A | 138 | -0.275 | 40.615 | 66.826 | 1.00 | 20.22 |
|    | ATOM | 1072 | N   | HIS | A | 139 | 1.718  | 43.223 | 62.265 | 1.00 | 24.05 |
| 60 | ATOM | 1073 | CA  | HIS | A | 139 | 1.322  | 44.511 | 61.824 | 1.00 | 24.05 |
|    | ATOM | 1074 | C   | HIS | A | 139 | 0.982  | 44.579 | 60.351 | 1.00 | 34.40 |
|    | ATOM | 1075 | O   | HIS | A | 139 | 0.539  | 45.625 | 59.888 | 1.00 | 35.89 |
|    | ATOM | 1076 | CB  | HIS | A | 139 | 2.439  | 45.519 | 62.173 | 1.00 | 24.63 |
|    | ATOM | 1077 | CG  | HIS | A | 139 | 2.689  | 45.619 | 63.657 | 1.00 | 27.97 |
|    | ATOM | 1078 | ND1 | HIS | A | 139 | 1.679  | 45.970 | 64.571 | 1.00 | 27.75 |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
|    | ATOM | 1079 | CD2 | HIS | A | 139 | 3.835  | 45.437 | 64.356 | 1.00 | 28.42 |
|    | ATOM | 1080 | CE1 | HIS | A | 139 | 2.222  | 45.983 | 65.770 | 1.00 | 26.19 |
|    | ATOM | 1081 | NE2 | HIS | A | 139 | 3.517  | 45.668 | 65.671 | 1.00 | 27.42 |
| 5  | ATOM | 1082 | N   | CYS | A | 140 | 1.181  | 43.490 | 59.598 | 1.00 | 30.28 |
|    | ATOM | 1083 | CA  | CYS | A | 140 | 0.832  | 43.517 | 58.181 | 1.00 | 28.08 |
|    | ATOM | 1084 | C   | CYS | A | 140 | -0.671 | 43.765 | 58.011 | 1.00 | 28.98 |
|    | ATOM | 1085 | O   | CYS | A | 140 | -1.111 | 44.449 | 57.066 | 1.00 | 30.00 |
|    | ATOM | 1086 | CB  | CYS | A | 140 | 1.181  | 42.213 | 57.447 | 1.00 | 28.82 |
| 10 | ATOM | 1087 | SG  | CYS | A | 140 | 1.330  | 42.483 | 55.661 | 1.00 | 34.37 |
|    | ATOM | 1088 | N   | ARG | A | 141 | -1.440 | 43.168 | 58.949 | 1.00 | 20.78 |
|    | ATOM | 1089 | CA  | ARG | A | 141 | -2.884 | 43.252 | 58.996 | 1.00 | 20.33 |
|    | ATOM | 1090 | C   | ARG | A | 141 | -3.286 | 44.684 | 59.003 | 1.00 | 32.37 |
|    | ATOM | 1091 | O   | ARG | A | 141 | -4.355 | 45.032 | 58.510 | 1.00 | 35.81 |
| 15 | ATOM | 1092 | CB  | ARG | A | 141 | -3.557 | 42.498 | 60.156 | 1.00 | 14.60 |
|    | ATOM | 1093 | CG  | ARG | A | 141 | -3.081 | 42.891 | 61.568 | 1.00 | 20.94 |
|    | ATOM | 1094 | CD  | ARG | A | 141 | -3.576 | 41.978 | 62.715 | 1.00 | 19.99 |
|    | ATOM | 1095 | NE  | ARG | A | 141 | -2.911 | 40.690 | 62.786 | 1.00 | 18.24 |
|    | ATOM | 1096 | CZ  | ARG | A | 141 | -3.140 | 39.707 | 63.648 | 1.00 | 18.77 |
| 20 | ATOM | 1097 | NH1 | ARG | A | 141 | -4.029 | 39.739 | 64.634 | 1.00 | 20.76 |
|    | ATOM | 1098 | NH2 | ARG | A | 141 | -2.415 | 38.640 | 63.508 | 1.00 | 24.20 |
|    | ATOM | 1099 | N   | ALA | A | 142 | -2.408 | 45.511 | 59.580 | 1.00 | 28.35 |
|    | ATOM | 1100 | CA  | ALA | A | 142 | -2.668 | 46.940 | 59.657 | 1.00 | 27.60 |
|    | ATOM | 1101 | C   | ALA | A | 142 | -2.369 | 47.652 | 58.345 | 1.00 | 34.33 |
| 25 | ATOM | 1102 | O   | ALA | A | 142 | -2.620 | 48.835 | 58.203 | 1.00 | 34.36 |
|    | ATOM | 1103 | CB  | ALA | A | 142 | -1.994 | 47.616 | 60.843 | 1.00 | 27.67 |
|    | ATOM | 1104 | N   | ILE | A | 143 | -1.824 | 46.922 | 57.382 | 1.00 | 32.39 |
|    | ATOM | 1105 | CA  | ILE | A | 143 | -1.537 | 47.499 | 56.099 | 1.00 | 30.38 |
|    | ATOM | 1106 | C   | ILE | A | 143 | -2.520 | 46.994 | 55.067 | 1.00 | 37.79 |
| 30 | ATOM | 1107 | O   | ILE | A | 143 | -2.885 | 47.709 | 54.152 | 1.00 | 42.65 |
|    | ATOM | 1108 | CB  | ILE | A | 143 | -0.142 | 47.228 | 55.613 | 1.00 | 32.06 |
|    | ATOM | 1109 | CG1 | ILE | A | 143 | 0.827  | 48.062 | 56.414 | 1.00 | 31.71 |
|    | ATOM | 1110 | CG2 | ILE | A | 143 | -0.074 | 47.654 | 54.143 | 1.00 | 34.02 |
|    | ATOM | 1111 | CD1 | ILE | A | 143 | 2.258  | 47.774 | 55.988 | 1.00 | 42.10 |
| 35 | ATOM | 1112 | N   | LEU | A | 144 | -2.939 | 45.749 | 55.218 | 1.00 | 32.50 |
|    | ATOM | 1113 | CA  | LEU | A | 144 | -3.873 | 45.142 | 54.291 | 1.00 | 32.36 |
|    | ATOM | 1114 | C   | LEU | A | 144 | -4.435 | 43.838 | 54.849 | 1.00 | 40.36 |
|    | ATOM | 1115 | O   | LEU | A | 144 | -3.959 | 43.278 | 55.852 | 1.00 | 33.27 |
|    | ATOM | 1116 | CB  | LEU | A | 144 | -3.250 | 44.936 | 52.894 | 1.00 | 31.58 |
| 40 | ATOM | 1117 | CG  | LEU | A | 144 | -1.923 | 44.170 | 52.917 | 1.00 | 33.31 |
|    | ATOM | 1118 | CD1 | LEU | A | 144 | -2.147 | 42.770 | 52.352 | 1.00 | 32.07 |
|    | ATOM | 1119 | CD2 | LEU | A | 144 | -0.836 | 44.897 | 52.110 | 1.00 | 28.67 |
|    | ATOM | 1120 | N   | PRO | A | 145 | -5.490 | 43.347 | 54.213 | 1.00 | 40.02 |
|    | ATOM | 1121 | CA  | PRO | A | 145 | -6.080 | 42.129 | 54.715 | 1.00 | 37.86 |
| 45 | ATOM | 1122 | C   | PRO | A | 145 | -5.264 | 40.941 | 54.286 | 1.00 | 37.87 |
|    | ATOM | 1123 | O   | PRO | A | 145 | -4.819 | 40.831 | 53.144 | 1.00 | 35.27 |
|    | ATOM | 1124 | CB  | PRO | A | 145 | -7.530 | 42.080 | 54.220 | 1.00 | 38.81 |
|    | ATOM | 1125 | CG  | PRO | A | 145 | -7.778 | 43.393 | 53.492 | 1.00 | 41.34 |
|    | ATOM | 1126 | CD  | PRO | A | 145 | -6.432 | 44.093 | 53.341 | 1.00 | 36.69 |
| 50 | ATOM | 1127 | N   | CYS | A | 146 | -5.041 | 40.056 | 55.233 | 1.00 | 36.18 |
|    | ATOM | 1128 | CA  | CYS | A | 146 | -4.250 | 38.882 | 54.958 | 1.00 | 35.60 |
|    | ATOM | 1129 | C   | CYS | A | 146 | -4.358 | 37.859 | 56.069 | 1.00 | 33.04 |
|    | ATOM | 1130 | O   | CYS | A | 146 | -5.067 | 38.062 | 57.050 | 1.00 | 30.78 |
|    | ATOM | 1131 | CB  | CYS | A | 146 | -2.761 | 39.287 | 54.813 | 1.00 | 36.08 |
| 55 | ATOM | 1132 | SG  | CYS | A | 146 | -2.087 | 40.108 | 56.302 | 1.00 | 39.43 |
|    | ATOM | 1133 | N   | GLN | A | 147 | -3.637 | 36.755 | 55.883 | 1.00 | 29.33 |
|    | ATOM | 1134 | CA  | GLN | A | 147 | -3.517 | 35.703 | 56.875 | 1.00 | 29.71 |
|    | ATOM | 1135 | C   | GLN | A | 147 | -2.254 | 36.131 | 57.628 | 1.00 | 38.75 |
|    | ATOM | 1136 | O   | GLN | A | 147 | -1.141 | 35.926 | 57.135 | 1.00 | 40.79 |
| 60 | ATOM | 1137 | CB  | GLN | A | 147 | -3.322 | 34.352 | 56.206 | 1.00 | 28.99 |
|    | ATOM | 1138 | CG  | GLN | A | 147 | -4.672 | 33.707 | 55.894 | 1.00 | 25.73 |
|    | ATOM | 1139 | CD  | GLN | A | 147 | -4.562 | 32.532 | 54.960 | 1.00 | 39.92 |
|    | ATOM | 1140 | OE1 | GLN | A | 147 | -4.217 | 32.668 | 53.775 | 1.00 | 43.89 |
|    | ATOM | 1141 | NE2 | GLN | A | 147 | -4.828 | 31.368 | 55.499 | 1.00 | 26.36 |
|    | ATOM | 1142 | N   | ASP | A | 148 | -2.425 | 36.834 | 58.765 | 1.00 | 32.68 |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
|    | ATOM | 1143 | CA  | ASP | A | 148 | -1.287 | 37.362 | 59.474 | 1.00 | 33.50 |
|    | ATOM | 1144 | C   | ASP | A | 148 | -0.629 | 36.377 | 60.371 | 1.00 | 33.13 |
|    | ATOM | 1145 | O   | ASP | A | 148 | -0.622 | 36.563 | 61.584 | 1.00 | 31.30 |
| 5  | ATOM | 1146 | CB  | ASP | A | 148 | -1.633 | 38.642 | 60.253 | 1.00 | 37.78 |
|    | ATOM | 1147 | CG  | ASP | A | 148 | -0.535 | 39.666 | 60.332 | 1.00 | 45.10 |
|    | ATOM | 1148 | OD1 | ASP | A | 148 | 0.564  | 39.540 | 59.836 | 1.00 | 47.89 |
|    | ATOM | 1149 | OD2 | ASP | A | 148 | -0.913 | 40.737 | 60.952 | 1.00 | 48.63 |
|    | ATOM | 1150 | N   | THR | A | 149 | -0.080 | 35.345 | 59.742 | 1.00 | 29.15 |
| 10 | ATOM | 1151 | CA  | THR | A | 149 | 0.584  | 34.251 | 60.422 | 1.00 | 28.25 |
|    | ATOM | 1152 | C   | THR | A | 149 | 1.805  | 33.831 | 59.625 | 1.00 | 34.92 |
|    | ATOM | 1153 | O   | THR | A | 149 | 1.757  | 33.764 | 58.410 | 1.00 | 34.47 |
|    | ATOM | 1154 | CB  | THR | A | 149 | -0.403 | 33.087 | 60.674 | 1.00 | 24.79 |
|    | ATOM | 1155 | OG1 | THR | A | 149 | 0.241  | 32.059 | 61.352 | 1.00 | 37.15 |
| 15 | ATOM | 1156 | CG2 | THR | A | 149 | -0.905 | 32.527 | 59.345 | 1.00 | 26.56 |
|    | ATOM | 1157 | N   | PRO | A | 150 | 2.910  | 33.575 | 60.323 | 1.00 | 34.69 |
|    | ATOM | 1158 | CA  | PRO | A | 150 | 4.142  | 33.217 | 59.659 | 1.00 | 31.06 |
|    | ATOM | 1159 | C   | PRO | A | 150 | 4.087  | 31.813 | 59.131 | 1.00 | 36.66 |
|    | ATOM | 1160 | O   | PRO | A | 150 | 4.995  | 31.356 | 58.450 | 1.00 | 36.37 |
| 20 | ATOM | 1161 | CB  | PRO | A | 150 | 5.245  | 33.327 | 60.712 | 1.00 | 31.18 |
|    | ATOM | 1162 | CG  | PRO | A | 150 | 4.570  | 33.471 | 62.077 | 1.00 | 36.95 |
|    | ATOM | 1163 | CD  | PRO | A | 150 | 3.078  | 33.589 | 61.823 | 1.00 | 34.62 |
|    | ATOM | 1164 | N   | SER | A | 151 | 2.992  | 31.150 | 59.452 | 1.00 | 31.62 |
|    | ATOM | 1165 | CA  | SER | A | 151 | 2.778  | 29.791 | 59.029 | 1.00 | 27.35 |
| 25 | ATOM | 1166 | C   | SER | A | 151 | 2.357  | 29.738 | 57.564 | 1.00 | 32.97 |
|    | ATOM | 1167 | O   | SER | A | 151 | 2.344  | 28.703 | 56.928 | 1.00 | 34.25 |
|    | ATOM | 1168 | CB  | SER | A | 151 | 1.714  | 29.203 | 59.905 | 1.00 | 25.95 |
|    | ATOM | 1169 | OG  | SER | A | 151 | 0.483  | 29.685 | 59.439 | 1.00 | 49.35 |
|    | ATOM | 1170 | N   | VAL | A | 152 | 1.997  | 30.887 | 57.024 | 1.00 | 34.36 |
| 30 | ATOM | 1171 | CA  | VAL | A | 152 | 1.595  | 31.015 | 55.623 | 1.00 | 33.74 |
|    | ATOM | 1172 | C   | VAL | A | 152 | 2.705  | 31.764 | 54.847 | 1.00 | 37.45 |
|    | ATOM | 1173 | O   | VAL | A | 152 | 3.295  | 32.761 | 55.313 | 1.00 | 37.63 |
|    | ATOM | 1174 | CB  | VAL | A | 152 | 0.203  | 31.697 | 55.427 | 1.00 | 32.61 |
|    | ATOM | 1175 | CG1 | VAL | A | 152 | -0.184 | 31.767 | 53.963 | 1.00 | 31.50 |
| 35 | ATOM | 1176 | CG2 | VAL | A | 152 | -0.915 | 30.975 | 56.149 | 1.00 | 31.29 |
|    | ATOM | 1177 | N   | LYS | A | 153 | 2.999  | 31.289 | 53.654 | 1.00 | 26.98 |
|    | ATOM | 1178 | CA  | LYS | A | 153 | 4.002  | 31.927 | 52.866 | 1.00 | 25.81 |
|    | ATOM | 1179 | C   | LYS | A | 153 | 3.469  | 32.141 | 51.473 | 1.00 | 33.94 |
|    | ATOM | 1180 | O   | LYS | A | 153 | 2.826  | 31.251 | 50.936 | 1.00 | 32.91 |
| 40 | ATOM | 1181 | CB  | LYS | A | 153 | 5.252  | 31.091 | 52.841 | 1.00 | 24.70 |
|    | ATOM | 1182 | CG  | LYS | A | 153 | 6.383  | 31.760 | 53.583 | 1.00 | 34.68 |
|    | ATOM | 1183 | CD  | LYS | A | 153 | 7.641  | 30.893 | 53.616 | 1.00 | 39.37 |
|    | ATOM | 1184 | CE  | LYS | A | 153 | 8.121  | 30.506 | 55.015 | 1.00 | 29.09 |
|    | ATOM | 1185 | NZ  | LYS | A | 153 | 9.556  | 30.152 | 55.112 | 1.00 | 26.03 |
| 45 | ATOM | 1186 | N   | LEU | A | 154 | 3.732  | 33.321 | 50.896 | 1.00 | 32.13 |
|    | ATOM | 1187 | CA  | LEU | A | 154 | 3.285  | 33.639 | 49.544 | 1.00 | 30.67 |
|    | ATOM | 1188 | C   | LEU | A | 154 | 4.279  | 34.475 | 48.789 | 1.00 | 40.67 |
|    | ATOM | 1189 | O   | LEU | A | 154 | 5.264  | 35.000 | 49.344 | 1.00 | 42.56 |
|    | ATOM | 1190 | CB  | LEU | A | 154 | 1.966  | 34.432 | 49.515 | 1.00 | 30.10 |
| 50 | ATOM | 1191 | CG  | LEU | A | 154 | 2.084  | 35.793 | 50.207 | 1.00 | 35.20 |
|    | ATOM | 1192 | CD1 | LEU | A | 154 | 0.989  | 36.716 | 49.690 | 1.00 | 37.21 |
|    | ATOM | 1193 | CD2 | LEU | A | 154 | 1.934  | 35.608 | 51.715 | 1.00 | 33.07 |
|    | ATOM | 1194 | N   | THR | A | 155 | 3.963  | 34.610 | 47.499 | 1.00 | 37.82 |
|    | ATOM | 1195 | CA  | THR | A | 155 | 4.728  | 35.449 | 46.596 | 1.00 | 38.44 |
| 55 | ATOM | 1196 | C   | THR | A | 155 | 3.934  | 36.730 | 46.389 | 1.00 | 41.52 |
|    | ATOM | 1197 | O   | THR | A | 155 | 2.738  | 36.775 | 46.674 | 1.00 | 43.95 |
|    | ATOM | 1198 | CB  | THR | A | 155 | 5.041  | 34.814 | 45.230 | 1.00 | 36.99 |
|    | ATOM | 1199 | OG1 | THR | A | 155 | 3.886  | 34.281 | 44.584 | 1.00 | 32.59 |
|    | ATOM | 1200 | CG2 | THR | A | 155 | 6.133  | 33.790 | 45.404 | 1.00 | 18.24 |
| 60 | ATOM | 1201 | N   | TYR | A | 156 | 4.563  | 37.768 | 45.892 | 1.00 | 33.87 |
|    | ATOM | 1202 | CA  | TYR | A | 156 | 3.835  | 39.003 | 45.683 | 1.00 | 32.49 |
|    | ATOM | 1203 | C   | TYR | A | 156 | 4.509  | 39.922 | 44.717 | 1.00 | 37.91 |
|    | ATOM | 1204 | O   | TYR | A | 156 | 5.725  | 39.940 | 44.562 | 1.00 | 39.04 |
|    | ATOM | 1205 | CB  | TYR | A | 156 | 3.534  | 39.795 | 46.983 | 1.00 | 31.16 |
|    | ATOM | 1206 | CG  | TYR | A | 156 | 4.642  | 40.731 | 47.471 | 1.00 | 28.94 |



|    |      |      |     |     |   |     |       |        |        |      |        |
|----|------|------|-----|-----|---|-----|-------|--------|--------|------|--------|
|    | ATOM | 1207 | CD1 | TYR | A | 156 | 4.817 | 42.021 | 46.969 | 1.00 | 30.33  |
|    | ATOM | 1208 | CD2 | TYR | A | 156 | 5.525 | 40.303 | 48.465 | 1.00 | 30.43  |
|    | ATOM | 1209 | CE1 | TYR | A | 156 | 5.829 | 42.853 | 47.459 | 1.00 | 36.89  |
| 5  | ATOM | 1210 | CE2 | TYR | A | 156 | 6.553 | 41.104 | 48.960 | 1.00 | 31.47  |
|    | ATOM | 1211 | CZ  | TYR | A | 156 | 6.690 | 42.396 | 48.462 | 1.00 | 43.34  |
|    | ATOM | 1212 | OH  | TYR | A | 156 | 7.701 | 43.180 | 48.956 | 1.00 | 36.86  |
|    | ATOM | 1213 | N   | THR | A | 157 | 3.657 | 40.689 | 44.101 | 1.00 | 36.75  |
|    | ATOM | 1214 | CA  | THR | A | 157 | 4.036 | 41.691 | 43.171 | 1.00 | 38.49  |
| 10 | ATOM | 1215 | C   | THR | A | 157 | 3.346 | 42.942 | 43.611 | 1.00 | 42.61  |
|    | ATOM | 1216 | O   | THR | A | 157 | 2.228 | 42.913 | 44.143 | 1.00 | 38.45  |
|    | ATOM | 1217 | CB  | THR | A | 157 | 3.631 | 41.316 | 41.751 | 1.00 | 39.73  |
|    | ATOM | 1218 | OG1 | THR | A | 157 | 2.380 | 40.655 | 41.803 | 1.00 | 55.71  |
|    | ATOM | 1219 | CG2 | THR | A | 157 | 4.680 | 40.370 | 41.212 | 1.00 | 26.71  |
| 15 | ATOM | 1220 | N   | ALA | A | 158 | 4.037 | 44.025 | 43.404 | 1.00 | 41.36  |
|    | ATOM | 1221 | CA  | ALA | A | 158 | 3.488 | 45.273 | 43.789 | 1.00 | 41.08  |
|    | ATOM | 1222 | C   | ALA | A | 158 | 3.869 | 46.401 | 42.839 | 1.00 | 50.77  |
|    | ATOM | 1223 | O   | ALA | A | 158 | 4.919 | 46.390 | 42.179 | 1.00 | 53.47  |
|    | ATOM | 1224 | CB  | ALA | A | 158 | 3.910 | 45.570 | 45.212 | 1.00 | 39.87  |
| 20 | ATOM | 1225 | N   | GLU | A | 159 | 2.974 | 47.376 | 42.788 | 1.00 | 43.90  |
|    | ATOM | 1226 | CA  | GLU | A | 159 | 3.107 | 48.604 | 42.023 | 1.00 | 42.27  |
|    | ATOM | 1227 | C   | GLU | A | 159 | 2.451 | 49.705 | 42.843 | 1.00 | 42.17  |
|    | ATOM | 1228 | O   | GLU | A | 159 | 1.257 | 49.630 | 43.227 | 1.00 | 41.00  |
|    | ATOM | 1229 | CB  | GLU | A | 159 | 2.641 | 48.521 | 40.571 | 1.00 | 43.72  |
| 25 | ATOM | 1230 | CG  | GLU | A | 159 | 1.943 | 47.197 | 40.255 | 1.00 | 62.90  |
|    | ATOM | 1231 | CD  | GLU | A | 159 | 1.502 | 47.156 | 38.835 | 1.00 | 91.28  |
|    | ATOM | 1232 | OE1 | GLU | A | 159 | 2.202 | 46.696 | 37.955 | 1.00 | 77.84  |
|    | ATOM | 1233 | OE2 | GLU | A | 159 | 0.322 | 47.707 | 38.644 | 1.00 | 100.00 |
|    | ATOM | 1234 | N   | VAL | A | 160 | 3.263 | 50.686 | 43.197 | 1.00 | 34.67  |
| 30 | ATOM | 1235 | CA  | VAL | A | 160 | 2.738 | 51.717 | 44.044 | 1.00 | 36.57  |
|    | ATOM | 1236 | C   | VAL | A | 160 | 3.024 | 53.091 | 43.533 | 1.00 | 43.02  |
|    | ATOM | 1237 | O   | VAL | A | 160 | 4.121 | 53.380 | 43.050 | 1.00 | 42.71  |
|    | ATOM | 1238 | CB  | VAL | A | 160 | 3.180 | 51.530 | 45.500 | 1.00 | 40.73  |
|    | ATOM | 1239 | CG1 | VAL | A | 160 | 3.988 | 50.239 | 45.644 | 1.00 | 38.56  |
| 35 | ATOM | 1240 | CG2 | VAL | A | 160 | 4.006 | 52.728 | 45.963 | 1.00 | 40.46  |
|    | ATOM | 1241 | N   | SER | A | 161 | 2.002 | 53.922 | 43.653 | 1.00 | 41.79  |
|    | ATOM | 1242 | CA  | SER | A | 161 | 2.076 | 55.292 | 43.185 | 1.00 | 42.07  |
|    | ATOM | 1243 | C   | SER | A | 161 | 2.532 | 56.204 | 44.270 | 1.00 | 44.28  |
|    | ATOM | 1244 | O   | SER | A | 161 | 2.047 | 56.121 | 45.403 | 1.00 | 43.60  |
| 40 | ATOM | 1245 | CB  | SER | A | 161 | 0.751 | 55.801 | 42.635 | 1.00 | 43.32  |
|    | ATOM | 1246 | OG  | SER | A | 161 | 0.971 | 56.850 | 41.726 | 1.00 | 49.40  |
|    | ATOM | 1247 | N   | VAL | A | 162 | 3.447 | 57.080 | 43.896 | 1.00 | 36.49  |
|    | ATOM | 1248 | CA  | VAL | A | 162 | 3.979 | 58.019 | 44.838 | 1.00 | 34.99  |
|    | ATOM | 1249 | C   | VAL | A | 162 | 4.273 | 59.319 | 44.148 | 1.00 | 42.57  |
| 45 | ATOM | 1250 | O   | VAL | A | 162 | 4.470 | 59.354 | 42.932 | 1.00 | 44.41  |
|    | ATOM | 1251 | CB  | VAL | A | 162 | 5.300 | 57.498 | 45.402 | 1.00 | 35.97  |
|    | ATOM | 1252 | CG1 | VAL | A | 162 | 5.084 | 56.219 | 46.188 | 1.00 | 36.12  |
|    | ATOM | 1253 | CG2 | VAL | A | 162 | 6.222 | 57.194 | 44.239 | 1.00 | 35.42  |
|    | ATOM | 1254 | N   | PRO | A | 163 | 4.332 | 60.377 | 44.942 | 1.00 | 32.95  |
| 50 | ATOM | 1255 | CA  | PRO | A | 163 | 4.664 | 61.662 | 44.400 | 1.00 | 31.07  |
|    | ATOM | 1256 | C   | PRO | A | 163 | 5.966 | 61.496 | 43.652 | 1.00 | 39.67  |
|    | ATOM | 1257 | O   | PRO | A | 163 | 6.919 | 60.892 | 44.142 | 1.00 | 42.78  |
|    | ATOM | 1258 | CB  | PRO | A | 163 | 4.780 | 62.562 | 45.618 | 1.00 | 31.62  |
|    | ATOM | 1259 | CG  | PRO | A | 163 | 3.946 | 61.893 | 46.714 | 1.00 | 33.93  |
| 55 | ATOM | 1260 | CD  | PRO | A | 163 | 3.652 | 60.480 | 46.259 | 1.00 | 28.53  |
|    | ATOM | 1261 | N   | LYS | A | 164 | 5.962 | 61.978 | 42.436 | 1.00 | 38.52  |
|    | ATOM | 1262 | CA  | LYS | A | 164 | 7.086 | 61.860 | 41.539 | 1.00 | 39.97  |
|    | ATOM | 1263 | C   | LYS | A | 164 | 8.451 | 62.222 | 42.088 | 1.00 | 42.75  |
|    | ATOM | 1264 | O   | LYS | A | 164 | 9.453 | 61.708 | 41.593 | 1.00 | 44.47  |
| 60 | ATOM | 1265 | CB  | LYS | A | 164 | 6.828 | 62.479 | 40.177 | 1.00 | 44.67  |
|    | ATOM | 1266 | CG  | LYS | A | 164 | 6.004 | 63.758 | 40.257 | 1.00 | 78.05  |
|    | ATOM | 1267 | CD  | LYS | A | 164 | 6.651 | 64.918 | 39.497 | 1.00 | 100.00 |
|    | ATOM | 1268 | CE  | LYS | A | 164 | 6.016 | 66.289 | 39.772 | 1.00 | 100.00 |
|    | ATOM | 1269 | NZ  | LYS | A | 164 | 6.679 | 67.075 | 40.835 | 1.00 | 100.00 |
|    | ATOM | 1270 | N   | GLU | A | 165 | 8.519 | 63.097 | 43.082 | 1.00 | 37.25  |



|    |      |      |     |     |       |        |        |        |      |       |
|----|------|------|-----|-----|-------|--------|--------|--------|------|-------|
|    | ATOM | 1271 | CA  | GLU | A 165 | 9.814  | 63.489 | 43.665 | 1.00 | 39.56 |
|    | ATOM | 1272 | C   | GLU | A 165 | 10.333 | 62.462 | 44.677 | 1.00 | 46.39 |
|    | ATOM | 1273 | O   | GLU | A 165 | 11.531 | 62.318 | 44.927 | 1.00 | 48.93 |
| 5  | ATOM | 1274 | CB  | GLU | A 165 | 9.797  | 64.902 | 44.297 | 1.00 | 42.10 |
|    | ATOM | 1275 | CG  | GLU | A 165 | 8.602  | 65.156 | 45.257 | 1.00 | 58.16 |
|    | ATOM | 1276 | CD  | GLU | A 165 | 7.214  | 64.970 | 44.664 | 1.00 | 88.01 |
|    | ATOM | 1277 | OE1 | GLU | A 165 | 6.994  | 64.757 | 43.475 | 1.00 | 79.46 |
|    | ATOM | 1278 | OE2 | GLU | A 165 | 6.266  | 65.050 | 45.575 | 1.00 | 70.27 |
| 10 | ATOM | 1279 | N   | LEU | A 166 | 9.398  | 61.733 | 45.265 | 1.00 | 40.39 |
|    | ATOM | 1280 | CA  | LEU | A 166 | 9.696  | 60.733 | 46.254 | 1.00 | 36.56 |
|    | ATOM | 1281 | C   | LEU | A 166 | 9.934  | 59.377 | 45.640 | 1.00 | 47.57 |
|    | ATOM | 1282 | O   | LEU | A 166 | 9.366  | 59.080 | 44.581 | 1.00 | 52.86 |
|    | ATOM | 1283 | CB  | LEU | A 166 | 8.525  | 60.630 | 47.250 | 1.00 | 31.92 |
| 15 | ATOM | 1284 | CG  | LEU | A 166 | 8.315  | 61.912 | 48.057 | 1.00 | 29.18 |
|    | ATOM | 1285 | CD1 | LEU | A 166 | 7.363  | 61.590 | 49.189 | 1.00 | 25.96 |
|    | ATOM | 1286 | CD2 | LEU | A 166 | 9.635  | 62.467 | 48.622 | 1.00 | 23.78 |
|    | ATOM | 1287 | N   | VAL | A 167 | 10.769 | 58.564 | 46.328 | 1.00 | 34.75 |
| 20 | ATOM | 1288 | CA  | VAL | A 167 | 11.077 | 57.218 | 45.908 | 1.00 | 30.00 |
|    | ATOM | 1289 | C   | VAL | A 167 | 10.332 | 56.229 | 46.771 | 1.00 | 38.80 |
|    | ATOM | 1290 | O   | VAL | A 167 | 9.902  | 56.532 | 47.879 | 1.00 | 40.91 |
|    | ATOM | 1291 | CB  | VAL | A 167 | 12.549 | 56.860 | 46.048 | 1.00 | 31.28 |
|    | ATOM | 1292 | CG1 | VAL | A 167 | 12.854 | 55.542 | 45.329 | 1.00 | 28.20 |
|    | ATOM | 1293 | CG2 | VAL | A 167 | 13.456 | 57.964 | 45.565 | 1.00 | 31.06 |
| 25 | ATOM | 1294 | N   | ALA | A 168 | 10.217 | 55.019 | 46.257 | 1.00 | 36.46 |
|    | ATOM | 1295 | CA  | ALA | A 168 | 9.584  | 53.935 | 46.979 | 1.00 | 35.14 |
|    | ATOM | 1296 | C   | ALA | A 168 | 10.418 | 52.662 | 46.836 | 1.00 | 43.27 |
|    | ATOM | 1297 | O   | ALA | A 168 | 10.889 | 52.343 | 45.733 | 1.00 | 44.74 |
|    | ATOM | 1298 | CB  | ALA | A 168 | 8.149  | 53.700 | 46.550 | 1.00 | 34.20 |
| 30 | ATOM | 1299 | N   | LEU | A 169 | 10.603 | 51.960 | 47.975 | 1.00 | 35.27 |
|    | ATOM | 1300 | CA  | LEU | A 169 | 11.323 | 50.696 | 48.069 | 1.00 | 29.39 |
|    | ATOM | 1301 | C   | LEU | A 169 | 10.491 | 49.635 | 48.797 | 1.00 | 33.87 |
|    | ATOM | 1302 | O   | LEU | A 169 | 9.604  | 49.918 | 49.613 | 1.00 | 31.21 |
|    | ATOM | 1303 | CB  | LEU | A 169 | 12.721 | 50.835 | 48.656 | 1.00 | 28.62 |
| 35 | ATOM | 1304 | CG  | LEU | A 169 | 13.593 | 51.810 | 47.891 | 1.00 | 35.90 |
|    | ATOM | 1305 | CD1 | LEU | A 169 | 14.953 | 51.819 | 48.558 | 1.00 | 39.38 |
|    | ATOM | 1306 | CD2 | LEU | A 169 | 13.765 | 51.394 | 46.432 | 1.00 | 37.35 |
|    | ATOM | 1307 | N   | MET | A 170 | 10.758 | 48.381 | 48.479 | 1.00 | 34.23 |
|    | ATOM | 1308 | CA  | MET | A 170 | 10.012 | 47.291 | 49.069 | 1.00 | 31.07 |
| 40 | ATOM | 1309 | C   | MET | A 170 | 10.874 | 46.083 | 49.287 | 1.00 | 34.13 |
|    | ATOM | 1310 | O   | MET | A 170 | 11.995 | 45.973 | 48.775 | 1.00 | 35.20 |
|    | ATOM | 1311 | CB  | MET | A 170 | 8.842  | 46.882 | 48.154 | 1.00 | 31.95 |
|    | ATOM | 1312 | CG  | MET | A 170 | 7.751  | 47.934 | 48.116 | 1.00 | 33.13 |
|    | ATOM | 1313 | SD  | MET | A 170 | 6.105  | 47.253 | 47.815 | 1.00 | 34.54 |
| 45 | ATOM | 1314 | CE  | MET | A 170 | 5.820  | 46.349 | 49.363 | 1.00 | 32.25 |
|    | ATOM | 1315 | N   | SER | A 171 | 10.332 | 45.165 | 50.057 | 1.00 | 28.20 |
|    | ATOM | 1316 | CA  | SER | A 171 | 11.064 | 43.953 | 50.297 | 1.00 | 28.47 |
|    | ATOM | 1317 | C   | SER | A 171 | 10.929 | 43.054 | 49.049 | 1.00 | 32.01 |
|    | ATOM | 1318 | O   | SER | A 171 | 10.396 | 41.958 | 49.089 | 1.00 | 30.93 |
| 50 | ATOM | 1319 | CB  | SER | A 171 | 10.662 | 43.265 | 51.606 | 1.00 | 30.93 |
|    | ATOM | 1320 | OG  | SER | A 171 | 9.297  | 42.920 | 51.581 | 1.00 | 32.90 |
|    | ATOM | 1321 | N   | ALA | A 172 | 11.401 | 43.543 | 47.912 | 1.00 | 28.84 |
|    | ATOM | 1322 | CA  | ALA | A 172 | 11.286 | 42.773 | 46.691 | 1.00 | 29.48 |
|    | ATOM | 1323 | C   | ALA | A 172 | 12.241 | 43.258 | 45.644 | 1.00 | 37.63 |
| 55 | ATOM | 1324 | O   | ALA | A 172 | 13.060 | 44.147 | 45.881 | 1.00 | 35.07 |
|    | ATOM | 1325 | CB  | ALA | A 172 | 9.884  | 42.969 | 46.120 | 1.00 | 29.48 |
|    | ATOM | 1326 | N   | ILE | A 173 | 12.104 | 42.686 | 44.452 | 1.00 | 39.49 |
|    | ATOM | 1327 | CA  | ILE | A 173 | 12.966 | 43.120 | 43.382 | 1.00 | 38.64 |
|    | ATOM | 1328 | C   | ILE | A 173 | 12.418 | 44.343 | 42.648 | 1.00 | 44.83 |
| 60 | ATOM | 1329 | O   | ILE | A 173 | 11.269 | 44.394 | 42.193 | 1.00 | 40.97 |
|    | ATOM | 1330 | CB  | ILE | A 173 | 13.549 | 42.027 | 42.479 | 1.00 | 38.79 |
|    | ATOM | 1331 | CG1 | ILE | A 173 | 14.258 | 40.970 | 43.302 | 1.00 | 37.40 |
|    | ATOM | 1332 | CG2 | ILE | A 173 | 14.606 | 42.621 | 41.570 | 1.00 | 38.88 |
|    | ATOM | 1333 | CD1 | ILE | A 173 | 15.770 | 41.069 | 43.193 | 1.00 | 25.93 |
|    | ATOM | 1334 | N   | ARG | A 174 | 13.286 | 45.345 | 42.584 | 1.00 | 43.21 |



|    |      |      |     |     |   |     |        |        |        |      |        |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
|    | ATOM | 1335 | CA  | ARG | A | 174 | 12.997 | 46.567 | 41.917 | 1.00 | 42.34  |
|    | ATOM | 1336 | C   | ARG | A | 174 | 12.630 | 46.173 | 40.516 | 1.00 | 47.54  |
|    | ATOM | 1337 | O   | ARG | A | 174 | 13.478 | 45.667 | 39.770 | 1.00 | 42.08  |
| 5  | ATOM | 1338 | CB  | ARG | A | 174 | 14.254 | 47.422 | 41.937 | 1.00 | 42.47  |
|    | ATOM | 1339 | CG  | ARG | A | 174 | 14.231 | 48.450 | 43.075 | 1.00 | 53.40  |
|    | ATOM | 1340 | CD  | ARG | A | 174 | 15.617 | 48.917 | 43.515 | 1.00 | 33.80  |
|    | ATOM | 1341 | NE  | ARG | A | 174 | 16.036 | 50.083 | 42.756 | 1.00 | 53.32  |
|    | ATOM | 1342 | CZ  | ARG | A | 174 | 17.221 | 50.208 | 42.181 | 1.00 | 97.11  |
| 10 | ATOM | 1343 | NH1 | ARG | A | 174 | 18.132 | 49.243 | 42.266 | 1.00 | 100.00 |
|    | ATOM | 1344 | NH2 | ARG | A | 174 | 17.503 | 51.321 | 41.489 | 1.00 | 100.00 |
|    | ATOM | 1345 | N   | ASP | A | 175 | 11.356 | 46.356 | 40.195 | 1.00 | 51.12  |
|    | ATOM | 1346 | CA  | ASP | A | 175 | 10.858 | 45.981 | 38.882 | 1.00 | 53.89  |
|    | ATOM | 1347 | C   | ASP | A | 175 | 10.778 | 47.128 | 37.885 | 1.00 | 58.32  |
| 15 | ATOM | 1348 | O   | ASP | A | 175 | 10.455 | 46.901 | 36.727 | 1.00 | 56.00  |
|    | ATOM | 1349 | CB  | ASP | A | 175 | 9.533  | 45.186 | 38.948 | 1.00 | 57.16  |
|    | ATOM | 1350 | CG  | ASP | A | 175 | 9.196  | 44.446 | 37.675 | 1.00 | 81.25  |
|    | ATOM | 1351 | OD1 | ASP | A | 175 | 10.034 | 44.118 | 36.851 | 1.00 | 83.53  |
|    | ATOM | 1352 | OD2 | ASP | A | 175 | 7.910  | 44.176 | 37.558 | 1.00 | 92.45  |
| 20 | ATOM | 1353 | N   | GLY | A | 176 | 11.062 | 48.356 | 38.331 | 1.00 | 58.24  |
|    | ATOM | 1354 | CA  | GLY | A | 176 | 11.021 | 49.498 | 37.438 | 1.00 | 57.71  |
|    | ATOM | 1355 | C   | GLY | A | 176 | 9.969  | 50.546 | 37.773 | 1.00 | 58.98  |
|    | ATOM | 1356 | O   | GLY | A | 176 | 9.090  | 50.371 | 38.620 | 1.00 | 52.04  |
|    | ATOM | 1357 | N   | GLU | A | 177 | 10.110 | 51.649 | 37.050 | 1.00 | 63.72  |
| 25 | ATOM | 1358 | CA  | GLU | A | 177 | 9.267  | 52.812 | 37.172 | 1.00 | 67.79  |
|    | ATOM | 1359 | C   | GLU | A | 177 | 8.874  | 53.388 | 35.817 | 1.00 | 86.22  |
|    | ATOM | 1360 | O   | GLU | A | 177 | 9.614  | 53.364 | 34.830 | 1.00 | 91.14  |
|    | ATOM | 1361 | CB  | GLU | A | 177 | 9.986  | 53.902 | 38.006 | 1.00 | 68.25  |
|    | ATOM | 1362 | CG  | GLU | A | 177 | 11.432 | 54.145 | 37.519 | 1.00 | 71.58  |
| 30 | ATOM | 1363 | CD  | GLU | A | 177 | 12.183 | 55.088 | 38.404 | 1.00 | 85.08  |
|    | ATOM | 1364 | OE1 | GLU | A | 177 | 13.045 | 54.733 | 39.198 | 1.00 | 100.00 |
|    | ATOM | 1365 | OE2 | GLU | A | 177 | 11.765 | 56.316 | 38.264 | 1.00 | 56.71  |
|    | ATOM | 1366 | N   | THR | A | 178 | 7.671  | 53.924 | 35.835 | 1.00 | 84.76  |
|    | ATOM | 1367 | CA  | THR | A | 178 | 6.684  | 54.686 | 35.042 | 1.00 | 84.81  |
| 35 | ATOM | 1368 | C   | THR | A | 178 | 6.024  | 55.810 | 35.855 | 1.00 | 90.37  |
|    | ATOM | 1369 | O   | THR | A | 178 | 5.664  | 55.655 | 36.996 | 1.00 | 91.10  |
|    | ATOM | 1370 | CB  | THR | A | 178 | 5.618  | 53.713 | 34.561 | 1.00 | 89.82  |
|    | ATOM | 1371 | OG1 | THR | A | 178 | 5.283  | 52.830 | 35.636 | 1.00 | 80.25  |
|    | ATOM | 1372 | CG2 | THR | A | 178 | 6.161  | 52.898 | 33.396 | 1.00 | 93.46  |
| 40 | ATOM | 1373 | N   | PRO | A | 179 | 5.921  | 56.984 | 35.217 | 1.00 | 87.05  |
|    | ATOM | 1374 | CA  | PRO | A | 179 | 5.365  | 58.187 | 35.845 | 1.00 | 86.61  |
|    | ATOM | 1375 | C   | PRO | A | 179 | 3.857  | 58.419 | 35.531 | 1.00 | 89.04  |
|    | ATOM | 1376 | O   | PRO | A | 179 | 3.444  | 59.516 | 35.140 | 1.00 | 91.15  |
|    | ATOM | 1377 | CB  | PRO | A | 179 | 6.176  | 59.345 | 35.301 | 1.00 | 88.63  |
| 45 | ATOM | 1378 | CG  | PRO | A | 179 | 6.657  | 58.947 | 33.895 | 1.00 | 92.62  |
|    | ATOM | 1379 | CD  | PRO | A | 179 | 6.426  | 57.345 | 33.902 | 1.00 | 87.63  |
|    | ATOM | 1380 | N   | ASP | A | 180 | 3.020  | 57.347 | 35.694 | 1.00 | 82.31  |
|    | ATOM | 1381 | CA  | ASP | A | 180 | 1.616  | 57.568 | 35.310 | 1.00 | 81.19  |
|    | ATOM | 1382 | C   | ASP | A | 180 | 0.629  | 56.743 | 36.166 | 1.00 | 90.72  |
| 50 | ATOM | 1383 | O   | ASP | A | 180 | 0.533  | 55.519 | 36.072 | 1.00 | 91.13  |
|    | ATOM | 1384 | CB  | ASP | A | 180 | 1.458  | 57.196 | 33.827 | 1.00 | 82.12  |
|    | ATOM | 1385 | CG  | ASP | A | 180 | 0.087  | 57.651 | 33.327 | 1.00 | 95.94  |
|    | ATOM | 1386 | OD1 | ASP | A | 180 | -0.155 | 58.858 | 33.337 | 1.00 | 100.00 |
|    | ATOM | 1387 | OD2 | ASP | A | 180 | -0.714 | 56.801 | 32.946 | 1.00 | 94.36  |
| 55 | ATOM | 1388 | N   | PRO | A | 181 | -0.060 | 57.456 | 37.086 | 1.00 | 92.45  |
|    | ATOM | 1389 | CA  | PRO | A | 181 | -1.212 | 56.934 | 37.795 | 1.00 | 92.02  |
|    | ATOM | 1390 | C   | PRO | A | 181 | -2.519 | 57.566 | 37.284 | 1.00 | 100.00 |
|    | ATOM | 1391 | O   | PRO | A | 181 | -2.605 | 58.114 | 36.192 | 1.00 | 100.00 |
|    | ATOM | 1392 | CB  | PRO | A | 181 | -1.014 | 57.340 | 39.210 | 1.00 | 92.48  |
| 60 | ATOM | 1393 | CG  | PRO | A | 181 | -0.362 | 58.734 | 39.152 | 1.00 | 98.39  |
|    | ATOM | 1394 | CD  | PRO | A | 181 | 0.268  | 58.736 | 37.663 | 1.00 | 94.17  |
|    | ATOM | 1395 | N   | GLU | A | 182 | -3.567 | 57.456 | 38.141 | 1.00 | 100.00 |
|    | ATOM | 1396 | CA  | GLU | A | 182 | -4.822 | 58.161 | 37.876 | 1.00 | 98.21  |
|    | ATOM | 1397 | C   | GLU | A | 182 | -5.359 | 58.856 | 39.154 | 1.00 | 100.00 |
|    | ATOM | 1398 | O   | GLU | A | 182 | -6.404 | 59.497 | 39.167 | 1.00 | 99.44  |



|    |      |      |     |     |   |     |        |        |        |      |        |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
|    | ATOM | 1399 | CB  | GLU | A | 182 | -5.854 | 57.142 | 37.356 | 1.00 | 98.57  |
|    | ATOM | 1400 | CG  | GLU | A | 182 | -5.880 | 57.077 | 35.816 | 1.00 | 100.00 |
|    | ATOM | 1401 | CD  | GLU | A | 182 | -7.013 | 57.938 | 35.300 | 1.00 | 100.00 |
| 5  | ATOM | 1402 | OE1 | GLU | A | 182 | -7.817 | 58.385 | 36.105 | 1.00 | 100.00 |
|    | ATOM | 1403 | OE2 | GLU | A | 182 | -7.084 | 58.153 | 34.091 | 1.00 | 100.00 |
|    | ATOM | 1404 | N   | ASP | A | 183 | -4.607 | 58.672 | 40.265 | 1.00 | 98.63  |
|    | ATOM | 1405 | CA  | ASP | A | 183 | -5.021 | 59.257 | 41.552 | 1.00 | 97.49  |
|    | ATOM | 1406 | C   | ASP | A | 183 | -4.126 | 60.472 | 41.932 | 1.00 | 100.00 |
| 10 | ATOM | 1407 | O   | ASP | A | 183 | -3.464 | 61.061 | 41.079 | 1.00 | 100.00 |
|    | ATOM | 1408 | CB  | ASP | A | 183 | -4.946 | 58.144 | 42.619 | 1.00 | 98.36  |
|    | ATOM | 1409 | CG  | ASP | A | 183 | -3.612 | 57.409 | 42.547 | 1.00 | 100.00 |
|    | ATOM | 1410 | OD1 | ASP | A | 183 | -3.471 | 56.556 | 41.668 | 1.00 | 100.00 |
|    | ATOM | 1411 | OD2 | ASP | A | 183 | -2.741 | 57.688 | 43.364 | 1.00 | 100.00 |
| 15 | ATOM | 1412 | N   | PRO | A | 184 | -4.187 | 60.906 | 43.237 | 1.00 | 97.96  |
|    | ATOM | 1413 | CA  | PRO | A | 184 | -3.311 | 61.985 | 43.738 | 1.00 | 97.92  |
|    | ATOM | 1414 | C   | PRO | A | 184 | -1.865 | 61.528 | 44.071 | 1.00 | 97.89  |
|    | ATOM | 1415 | O   | PRO | A | 184 | -1.348 | 61.748 | 45.159 | 1.00 | 100.00 |
|    | ATOM | 1416 | CB  | PRO | A | 184 | -3.973 | 62.561 | 44.992 | 1.00 | 98.86  |
| 20 | ATOM | 1417 | CG  | PRO | A | 184 | -5.262 | 61.777 | 45.284 | 1.00 | 100.00 |
|    | ATOM | 1418 | CD  | PRO | A | 184 | -5.122 | 60.532 | 44.284 | 1.00 | 97.20  |
|    | ATOM | 1419 | N   | SER | A | 185 | -1.249 | 60.840 | 43.071 | 1.00 | 82.40  |
|    | ATOM | 1420 | CA  | SER | A | 185 | 0.196  | 60.496 | 43.086 | 1.00 | 75.26  |
|    | ATOM | 1421 | C   | SER | A | 185 | 0.748  | 60.563 | 41.623 | 1.00 | 71.84  |
| 25 | ATOM | 1422 | O   | SER | A | 185 | -0.006 | 60.525 | 40.670 | 1.00 | 77.97  |
|    | ATOM | 1423 | CB  | SER | A | 185 | 0.337  | 59.068 | 43.636 | 1.00 | 73.41  |
|    | ATOM | 1424 | OG  | SER | A | 185 | 0.672  | 59.109 | 45.027 | 1.00 | 63.60  |
|    | ATOM | 1425 | N   | ARG | A | 186 | 2.107  | 60.704 | 41.461 | 1.00 | 57.89  |
|    | ATOM | 1426 | CA  | ARG | A | 186 | 2.650  | 60.971 | 40.088 | 1.00 | 56.00  |
| 30 | ATOM | 1427 | C   | ARG | A | 186 | 3.725  | 59.943 | 39.633 | 1.00 | 59.64  |
|    | ATOM | 1428 | O   | ARG | A | 186 | 4.473  | 60.157 | 38.688 | 1.00 | 60.30  |
|    | ATOM | 1429 | CB  | ARG | A | 186 | 3.258  | 62.393 | 40.064 | 1.00 | 63.74  |
|    | ATOM | 1430 | CG  | ARG | A | 186 | 2.339  | 63.457 | 40.677 | 1.00 | 80.44  |
|    | ATOM | 1431 | CD  | ARG | A | 186 | 1.188  | 63.874 | 39.736 | 1.00 | 71.31  |
| 35 | ATOM | 1432 | NE  | ARG | A | 186 | 1.316  | 63.215 | 38.436 | 1.00 | 79.64  |
|    | ATOM | 1433 | CZ  | ARG | A | 186 | 0.185  | 62.862 | 37.784 | 1.00 | 95.30  |
|    | ATOM | 1434 | NH1 | ARG | A | 186 | -0.999 | 63.109 | 38.312 | 1.00 | 56.25  |
|    | ATOM | 1435 | NH2 | ARG | A | 186 | 0.276  | 62.232 | 36.603 | 1.00 | 89.98  |
|    | ATOM | 1436 | N   | LYS | A | 187 | 3.892  | 58.778 | 40.265 | 1.00 | 54.50  |
| 40 | ATOM | 1437 | CA  | LYS | A | 187 | 4.891  | 57.805 | 39.851 | 1.00 | 51.93  |
|    | ATOM | 1438 | C   | LYS | A | 187 | 4.506  | 56.436 | 40.276 | 1.00 | 52.96  |
|    | ATOM | 1439 | O   | LYS | A | 187 | 3.971  | 56.236 | 41.368 | 1.00 | 53.58  |
|    | ATOM | 1440 | CB  | LYS | A | 187 | 6.247  | 58.047 | 40.470 | 1.00 | 53.78  |
|    | ATOM | 1441 | CG  | LYS | A | 187 | 7.427  | 57.714 | 39.574 | 1.00 | 43.05  |
| 45 | ATOM | 1442 | CD  | LYS | A | 187 | 8.517  | 58.761 | 39.762 | 1.00 | 53.36  |
|    | ATOM | 1443 | CE  | LYS | A | 187 | 9.870  | 58.468 | 39.146 | 1.00 | 39.68  |
|    | ATOM | 1444 | NZ  | LYS | A | 187 | 10.795 | 59.601 | 39.341 | 1.00 | 40.19  |
|    | ATOM | 1445 | N   | ILE | A | 188 | 4.819  | 55.502 | 39.403 | 1.00 | 46.36  |
|    | ATOM | 1446 | CA  | ILE | A | 188 | 4.565  | 54.128 | 39.700 | 1.00 | 43.57  |
| 50 | ATOM | 1447 | C   | ILE | A | 188 | 5.824  | 53.311 | 39.851 | 1.00 | 42.64  |
|    | ATOM | 1448 | O   | ILE | A | 188 | 6.647  | 53.189 | 38.937 | 1.00 | 41.55  |
|    | ATOM | 1449 | CB  | ILE | A | 188 | 3.579  | 53.425 | 38.826 | 1.00 | 45.64  |
|    | ATOM | 1450 | CG1 | ILE | A | 188 | 2.193  | 54.021 | 39.047 | 1.00 | 45.82  |
|    | ATOM | 1451 | CG2 | ILE | A | 188 | 3.590  | 51.969 | 39.273 | 1.00 | 43.43  |
| 55 | ATOM | 1452 | CD1 | ILE | A | 188 | 1.448  | 53.505 | 40.276 | 1.00 | 62.08  |
|    | ATOM | 1453 | N   | TYR | A | 189 | 5.950  | 52.757 | 41.042 | 1.00 | 35.58  |
|    | ATOM | 1454 | CA  | TYR | A | 189 | 7.079  | 51.933 | 41.356 | 1.00 | 37.57  |
|    | ATOM | 1455 | C   | TYR | A | 189 | 6.652  | 50.465 | 41.359 | 1.00 | 44.89  |
|    | ATOM | 1456 | O   | TYR | A | 189 | 5.656  | 50.092 | 41.999 | 1.00 | 44.33  |
| 60 | ATOM | 1457 | CB  | TYR | A | 189 | 7.752  | 52.392 | 42.661 | 1.00 | 37.85  |
|    | ATOM | 1458 | CG  | TYR | A | 189 | 8.692  | 53.563 | 42.456 | 1.00 | 34.49  |
|    | ATOM | 1459 | CD1 | TYR | A | 189 | 9.968  | 53.375 | 41.930 | 1.00 | 35.93  |
|    | ATOM | 1460 | CD2 | TYR | A | 189 | 8.310  | 54.859 | 42.813 | 1.00 | 32.44  |
|    | ATOM | 1461 | CE1 | TYR | A | 189 | 10.843 | 54.449 | 41.753 | 1.00 | 36.88  |
|    | ATOM | 1462 | CE2 | TYR | A | 189 | 9.170  | 55.945 | 42.647 | 1.00 | 31.63  |



|    |      |      |     |     |   |     |        |        |        |      |        |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
|    | ATOM | 1463 | CZ  | TYR | A | 189 | 10.441 | 55.734 | 42.113 | 1.00 | 44.54  |
|    | ATOM | 1464 | OH  | TYR | A | 189 | 11.296 | 56.788 | 41.929 | 1.00 | 57.77  |
|    | ATOM | 1465 | N   | LYS | A | 190 | 7.413  | 49.651 | 40.608 | 1.00 | 42.91  |
| 5  | ATOM | 1466 | CA  | LYS | A | 190 | 7.173  | 48.210 | 40.420 | 1.00 | 42.22  |
|    | ATOM | 1467 | C   | LYS | A | 190 | 8.152  | 47.262 | 41.143 | 1.00 | 40.73  |
|    | ATOM | 1468 | O   | LYS | A | 190 | 9.398  | 47.400 | 41.093 | 1.00 | 35.69  |
|    | ATOM | 1469 | CB  | LYS | A | 190 | 7.007  | 47.839 | 38.944 | 1.00 | 45.87  |
|    | ATOM | 1470 | CG  | LYS | A | 190 | 5.735  | 48.403 | 38.306 | 1.00 | 71.08  |
| 10 | ATOM | 1471 | CD  | LYS | A | 190 | 5.758  | 48.384 | 36.779 | 1.00 | 84.62  |
|    | ATOM | 1472 | CE  | LYS | A | 190 | 4.386  | 48.157 | 36.147 | 1.00 | 100.00 |
|    | ATOM | 1473 | NZ  | LYS | A | 190 | 4.299  | 46.930 | 35.329 | 1.00 | 100.00 |
|    | ATOM | 1474 | N   | PHE | A | 191 | 7.539  | 46.264 | 41.812 | 1.00 | 35.01  |
|    | ATOM | 1475 | CA  | PHE | A | 191 | 8.276  | 45.304 | 42.592 | 1.00 | 31.57  |
|    | ATOM | 1476 | C   | PHE | A | 191 | 7.792  | 43.871 | 42.465 | 1.00 | 30.89  |
| 15 | ATOM | 1477 | O   | PHE | A | 191 | 6.603  | 43.584 | 42.377 | 1.00 | 25.06  |
|    | ATOM | 1478 | CB  | PHE | A | 191 | 8.217  | 45.734 | 44.080 | 1.00 | 32.11  |
|    | ATOM | 1479 | CG  | PHE | A | 191 | 8.570  | 47.190 | 44.372 | 1.00 | 29.24  |
|    | ATOM | 1480 | CD1 | PHE | A | 191 | 9.895  | 47.593 | 44.539 | 1.00 | 31.81  |
| 20 | ATOM | 1481 | CD2 | PHE | A | 191 | 7.565  | 48.147 | 44.508 | 1.00 | 30.17  |
|    | ATOM | 1482 | CE1 | PHE | A | 191 | 10.230 | 48.925 | 44.805 | 1.00 | 34.10  |
|    | ATOM | 1483 | CE2 | PHE | A | 191 | 7.866  | 49.483 | 44.776 | 1.00 | 33.69  |
|    | ATOM | 1484 | CZ  | PHE | A | 191 | 9.201  | 49.860 | 44.928 | 1.00 | 33.32  |
|    | ATOM | 1485 | N   | ILE | A | 192 | 8.764  | 42.961 | 42.505 | 1.00 | 35.75  |
|    | ATOM | 1486 | CA  | ILE | A | 192 | 8.525  | 41.520 | 42.415 | 1.00 | 37.02  |
| 25 | ATOM | 1487 | C   | ILE | A | 192 | 9.255  | 40.653 | 43.469 | 1.00 | 33.05  |
|    | ATOM | 1488 | O   | ILE | A | 192 | 10.489 | 40.672 | 43.593 | 1.00 | 30.73  |
|    | ATOM | 1489 | CB  | ILE | A | 192 | 8.850  | 40.970 | 41.025 | 1.00 | 42.45  |
|    | ATOM | 1490 | CG1 | ILE | A | 192 | 8.289  | 41.914 | 39.981 | 1.00 | 46.39  |
|    | ATOM | 1491 | CG2 | ILE | A | 192 | 8.251  | 39.567 | 40.859 | 1.00 | 44.02  |
| 30 | ATOM | 1492 | CD1 | ILE | A | 192 | 7.609  | 41.231 | 38.798 | 1.00 | 69.61  |
|    | ATOM | 1493 | N   | GLN | A | 193 | 8.459  | 39.864 | 44.195 | 1.00 | 27.51  |
|    | ATOM | 1494 | CA  | GLN | A | 193 | 8.954  | 38.908 | 45.177 | 1.00 | 32.05  |
|    | ATOM | 1495 | C   | GLN | A | 193 | 8.626  | 37.488 | 44.757 | 1.00 | 44.32  |
|    | ATOM | 1496 | O   | GLN | A | 193 | 7.583  | 36.926 | 45.120 | 1.00 | 43.11  |
| 35 | ATOM | 1497 | CB  | GLN | A | 193 | 8.502  | 39.100 | 46.638 | 1.00 | 33.44  |
|    | ATOM | 1498 | CG  | GLN | A | 193 | 9.285  | 38.203 | 47.632 | 1.00 | 22.34  |
|    | ATOM | 1499 | CD  | GLN | A | 193 | 10.824 | 38.337 | 47.636 | 1.00 | 48.52  |
|    | ATOM | 1500 | OE1 | GLN | A | 193 | 11.557 | 37.537 | 47.016 | 1.00 | 45.24  |
|    | ATOM | 1501 | NE2 | GLN | A | 193 | 11.326 | 39.330 | 48.373 | 1.00 | 24.82  |
| 40 | ATOM | 1502 | N   | LYS | A | 194 | 9.543  | 36.908 | 43.993 | 1.00 | 46.91  |
|    | ATOM | 1503 | CA  | LYS | A | 194 | 9.384  | 35.540 | 43.529 | 1.00 | 47.56  |
|    | ATOM | 1504 | C   | LYS | A | 194 | 9.456  | 34.524 | 44.666 | 1.00 | 49.56  |
|    | ATOM | 1505 | O   | LYS | A | 194 | 8.777  | 33.520 | 44.598 | 1.00 | 50.85  |
|    | ATOM | 1506 | CB  | LYS | A | 194 | 10.385 | 35.159 | 42.439 | 1.00 | 48.11  |
| 45 | ATOM | 1507 | CG  | LYS | A | 194 | 9.884  | 35.443 | 41.031 | 1.00 | 55.70  |
|    | ATOM | 1508 | CD  | LYS | A | 194 | 10.895 | 36.200 | 40.179 | 1.00 | 67.67  |
|    | ATOM | 1509 | CE  | LYS | A | 194 | 10.614 | 36.122 | 38.682 | 1.00 | 81.92  |
|    | ATOM | 1510 | NZ  | LYS | A | 194 | 11.284 | 37.185 | 37.910 | 1.00 | 88.34  |
|    | ATOM | 1511 | N   | VAL | A | 195 | 10.308 | 34.753 | 45.689 | 1.00 | 39.55  |
| 50 | ATOM | 1512 | CA  | VAL | A | 195 | 10.422 | 33.780 | 46.764 | 1.00 | 33.56  |
|    | ATOM | 1513 | C   | VAL | A | 195 | 9.261  | 33.862 | 47.698 | 1.00 | 35.67  |
|    | ATOM | 1514 | O   | VAL | A | 195 | 8.804  | 34.945 | 48.034 | 1.00 | 38.69  |
|    | ATOM | 1515 | CB  | VAL | A | 195 | 11.716 | 33.844 | 47.560 | 1.00 | 32.62  |
|    | ATOM | 1516 | CG1 | VAL | A | 195 | 11.849 | 32.539 | 48.310 | 1.00 | 32.40  |
| 55 | ATOM | 1517 | CG2 | VAL | A | 195 | 12.933 | 34.029 | 46.667 | 1.00 | 30.55  |
|    | ATOM | 1518 | N   | PRO | A | 196 | 8.770  | 32.717 | 48.126 | 1.00 | 27.75  |
|    | ATOM | 1519 | CA  | PRO | A | 196 | 7.653  | 32.757 | 49.038 | 1.00 | 26.18  |
|    | ATOM | 1520 | C   | PRO | A | 196 | 8.132  | 33.236 | 50.410 | 1.00 | 35.86  |
|    | ATOM | 1521 | O   | PRO | A | 196 | 9.185  | 32.809 | 50.899 | 1.00 | 35.43  |
| 60 | ATOM | 1522 | CB  | PRO | A | 196 | 7.022  | 31.359 | 49.044 | 1.00 | 26.04  |
|    | ATOM | 1523 | CG  | PRO | A | 196 | 7.856  | 30.472 | 48.113 | 1.00 | 27.79  |
|    | ATOM | 1524 | CD  | PRO | A | 196 | 8.964  | 31.352 | 47.546 | 1.00 | 25.40  |
|    | ATOM | 1525 | N   | ILE | A | 197 | 7.388  | 34.171 | 51.009 | 1.00 | 29.92  |
|    | ATOM | 1526 | CA  | ILE | A | 197 | 7.772  | 34.697 | 52.284 | 1.00 | 26.98  |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
|    | ATOM | 1527 | C   | ILE | A | 197 | 6.544  | 34.809 | 53.128 | 1.00 | 34.88 |
|    | ATOM | 1528 | O   | ILE | A | 197 | 5.444  | 34.788 | 52.606 | 1.00 | 29.68 |
|    | ATOM | 1529 | CB  | ILE | A | 197 | 8.334  | 36.100 | 52.094 | 1.00 | 27.90 |
| 5  | ATOM | 1530 | CG1 | ILE | A | 197 | 7.342  | 36.867 | 51.254 | 1.00 | 27.78 |
|    | ATOM | 1531 | CG2 | ILE | A | 197 | 9.659  | 36.091 | 51.337 | 1.00 | 28.12 |
|    | ATOM | 1532 | CD1 | ILE | A | 197 | 7.494  | 38.378 | 51.438 | 1.00 | 19.03 |
|    | ATOM | 1533 | N   | PRO | A | 198 | 6.743  | 34.936 | 54.447 | 1.00 | 36.02 |
|    | ATOM | 1534 | CA  | PRO | A | 198 | 5.647  | 35.110 | 55.410 | 1.00 | 31.31 |
| 10 | ATOM | 1535 | C   | PRO | A | 198 | 5.299  | 36.583 | 55.308 | 1.00 | 28.27 |
|    | ATOM | 1536 | O   | PRO | A | 198 | 6.212  | 37.391 | 55.115 | 1.00 | 22.70 |
|    | ATOM | 1537 | CB  | PRO | A | 198 | 6.252  | 34.849 | 56.794 | 1.00 | 31.17 |
|    | ATOM | 1538 | CG  | PRO | A | 198 | 7.768  | 34.768 | 56.615 | 1.00 | 34.94 |
|    | ATOM | 1539 | CD  | PRO | A | 198 | 8.057  | 34.706 | 55.122 | 1.00 | 32.99 |
| 15 | ATOM | 1540 | N   | CYS | A | 199 | 4.011  | 36.939 | 55.405 | 1.00 | 27.60 |
|    | ATOM | 1541 | CA  | CYS | A | 199 | 3.555  | 38.360 | 55.289 | 1.00 | 27.66 |
|    | ATOM | 1542 | C   | CYS | A | 199 | 4.255  | 39.390 | 56.187 | 1.00 | 30.13 |
|    | ATOM | 1543 | O   | CYS | A | 199 | 4.294  | 40.596 | 55.895 | 1.00 | 29.50 |
|    | ATOM | 1544 | CB  | CYS | A | 199 | 2.025  | 38.534 | 55.242 | 1.00 | 27.18 |
| 20 | ATOM | 1545 | SG  | CYS | A | 199 | 1.232  | 38.279 | 56.841 | 1.00 | 30.85 |
|    | ATOM | 1546 | N   | TYR | A | 200 | 4.847  | 38.903 | 57.270 | 1.00 | 26.15 |
|    | ATOM | 1547 | CA  | TYR | A | 200 | 5.538  | 39.798 | 58.123 | 1.00 | 28.28 |
|    | ATOM | 1548 | C   | TYR | A | 200 | 6.760  | 40.395 | 57.483 | 1.00 | 32.29 |
|    | ATOM | 1549 | O   | TYR | A | 200 | 7.359  | 41.286 | 58.036 | 1.00 | 31.56 |
| 25 | ATOM | 1550 | CB  | TYR | A | 200 | 5.844  | 39.215 | 59.489 | 1.00 | 30.59 |
|    | ATOM | 1551 | CG  | TYR | A | 200 | 6.989  | 38.272 | 59.568 | 1.00 | 28.28 |
|    | ATOM | 1552 | CD1 | TYR | A | 200 | 8.288  | 38.733 | 59.689 | 1.00 | 29.48 |
|    | ATOM | 1553 | CD2 | TYR | A | 200 | 6.756  | 36.903 | 59.475 | 1.00 | 27.55 |
|    | ATOM | 1554 | CE1 | TYR | A | 200 | 9.377  | 37.862 | 59.825 | 1.00 | 21.42 |
| 30 | ATOM | 1555 | CE2 | TYR | A | 200 | 7.838  | 36.015 | 59.595 | 1.00 | 27.41 |
|    | ATOM | 1556 | CZ  | TYR | A | 200 | 9.144  | 36.488 | 59.737 | 1.00 | 25.11 |
|    | ATOM | 1557 | OH  | TYR | A | 200 | 10.215 | 35.614 | 59.880 | 1.00 | 27.62 |
|    | ATOM | 1558 | N   | LEU | A | 201 | 7.113  | 39.897 | 56.313 | 1.00 | 31.66 |
|    | ATOM | 1559 | CA  | LEU | A | 201 | 8.278  | 40.378 | 55.579 | 1.00 | 29.49 |
| 35 | ATOM | 1560 | C   | LEU | A | 201 | 7.914  | 41.343 | 54.484 | 1.00 | 33.65 |
|    | ATOM | 1561 | O   | LEU | A | 201 | 8.767  | 41.737 | 53.686 | 1.00 | 35.31 |
|    | ATOM | 1562 | CB  | LEU | A | 201 | 9.225  | 39.275 | 55.035 | 1.00 | 27.04 |
|    | ATOM | 1563 | CG  | LEU | A | 201 | 9.697  | 38.271 | 56.071 | 1.00 | 27.42 |
|    | ATOM | 1564 | CD1 | LEU | A | 201 | 10.254 | 37.030 | 55.390 | 1.00 | 23.71 |
| 40 | ATOM | 1565 | CD2 | LEU | A | 201 | 10.764 | 38.913 | 56.957 | 1.00 | 30.55 |
|    | ATOM | 1566 | N   | ILE | A | 202 | 6.648  | 41.710 | 54.438 | 1.00 | 28.66 |
|    | ATOM | 1567 | CA  | ILE | A | 202 | 6.249  | 42.674 | 53.433 | 1.00 | 29.57 |
|    | ATOM | 1568 | C   | ILE | A | 202 | 6.636  | 44.074 | 53.951 | 1.00 | 40.28 |
|    | ATOM | 1569 | O   | ILE | A | 202 | 6.192  | 44.493 | 55.027 | 1.00 | 40.75 |
| 45 | ATOM | 1570 | CB  | ILE | A | 202 | 4.733  | 42.651 | 53.182 | 1.00 | 31.18 |
|    | ATOM | 1571 | CG1 | ILE | A | 202 | 4.250  | 41.429 | 52.405 | 1.00 | 28.21 |
|    | ATOM | 1572 | CG2 | ILE | A | 202 | 4.259  | 43.962 | 52.521 | 1.00 | 29.23 |
|    | ATOM | 1573 | CD1 | ILE | A | 202 | 2.724  | 41.288 | 52.449 | 1.00 | 23.01 |
|    | ATOM | 1574 | N   | ALA | A | 203 | 7.445  | 44.813 | 53.197 | 1.00 | 39.14 |
| 50 | ATOM | 1575 | CA  | ALA | A | 203 | 7.840  | 46.150 | 53.611 | 1.00 | 37.03 |
|    | ATOM | 1576 | C   | ALA | A | 203 | 7.819  | 47.159 | 52.482 | 1.00 | 34.32 |
|    | ATOM | 1577 | O   | ALA | A | 203 | 8.060  | 46.836 | 51.311 | 1.00 | 30.63 |
|    | ATOM | 1578 | CB  | ALA | A | 203 | 9.180  | 46.143 | 54.309 | 1.00 | 38.22 |
|    | ATOM | 1579 | N   | LEU | A | 204 | 7.514  | 48.388 | 52.910 | 1.00 | 33.64 |
| 55 | ATOM | 1580 | CA  | LEU | A | 204 | 7.388  | 49.604 | 52.102 | 1.00 | 32.56 |
|    | ATOM | 1581 | C   | LEU | A | 204 | 7.993  | 50.817 | 52.812 | 1.00 | 37.69 |
|    | ATOM | 1582 | O   | LEU | A | 204 | 7.854  | 51.037 | 54.034 | 1.00 | 32.66 |
|    | ATOM | 1583 | CB  | LEU | A | 204 | 5.906  | 49.929 | 51.718 | 1.00 | 29.74 |
|    | ATOM | 1584 | CG  | LEU | A | 204 | 5.706  | 51.182 | 50.855 | 1.00 | 29.64 |
| 60 | ATOM | 1585 | CD1 | LEU | A | 204 | 6.263  | 50.994 | 49.445 | 1.00 | 29.47 |
|    | ATOM | 1586 | CD2 | LEU | A | 204 | 4.222  | 51.515 | 50.750 | 1.00 | 33.50 |
|    | ATOM | 1587 | N   | VAL | A | 205 | 8.670  | 51.603 | 51.991 | 1.00 | 36.87 |
|    | ATOM | 1588 | CA  | VAL | A | 205 | 9.305  | 52.821 | 52.415 | 1.00 | 35.15 |
|    | ATOM | 1589 | C   | VAL | A | 205 | 9.224  | 53.795 | 51.284 | 1.00 | 38.41 |
|    | ATOM | 1590 | O   | VAL | A | 205 | 9.575  | 53.462 | 50.148 | 1.00 | 39.50 |



|    |      |      |     |     |   |     |        |        |        |      |        |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
|    | ATOM | 1591 | CB  | VAL | A | 205 | 10.769 | 52.651 | 52.804 | 1.00 | 36.06  |
|    | ATOM | 1592 | CG1 | VAL | A | 205 | 11.466 | 51.794 | 51.757 | 1.00 | 35.08  |
|    | ATOM | 1593 | CG2 | VAL | A | 205 | 11.432 | 54.020 | 52.833 | 1.00 | 35.98  |
| 5  | ATOM | 1594 | N   | VAL | A | 206 | 8.750  | 54.983 | 51.623 | 1.00 | 33.54  |
|    | ATOM | 1595 | CA  | VAL | A | 206 | 8.623  | 56.104 | 50.687 | 1.00 | 31.81  |
|    | ATOM | 1596 | C   | VAL | A | 206 | 9.300  | 57.343 | 51.249 | 1.00 | 31.62  |
|    | ATOM | 1597 | O   | VAL | A | 206 | 9.076  | 57.722 | 52.406 | 1.00 | 34.81  |
|    | ATOM | 1598 | CB  | VAL | A | 206 | 7.179  | 56.405 | 50.305 | 1.00 | 33.35  |
| 10 | ATOM | 1599 | CG1 | VAL | A | 206 | 7.129  | 57.243 | 49.029 | 1.00 | 33.44  |
|    | ATOM | 1600 | CG2 | VAL | A | 206 | 6.452  | 55.084 | 50.109 | 1.00 | 31.98  |
|    | ATOM | 1601 | N   | GLY | A | 207 | 10.130 | 57.959 | 50.431 | 1.00 | 24.94  |
|    | ATOM | 1602 | CA  | GLY | A | 207 | 10.807 | 59.168 | 50.861 | 1.00 | 27.25  |
|    | ATOM | 1603 | C   | GLY | A | 207 | 11.802 | 59.632 | 49.838 | 1.00 | 38.81  |
| 15 | ATOM | 1604 | O   | GLY | A | 207 | 12.046 | 58.966 | 48.840 | 1.00 | 39.82  |
|    | ATOM | 1605 | N   | ALA | A | 208 | 12.375 | 60.783 | 50.113 | 1.00 | 41.07  |
|    | ATOM | 1606 | CA  | ALA | A | 208 | 13.370 | 61.354 | 49.233 | 1.00 | 42.72  |
|    | ATOM | 1607 | C   | ALA | A | 208 | 14.660 | 60.550 | 49.356 | 1.00 | 49.10  |
|    | ATOM | 1608 | O   | ALA | A | 208 | 15.651 | 60.997 | 49.957 | 1.00 | 51.30  |
| 20 | ATOM | 1609 | CB  | ALA | A | 208 | 13.605 | 62.810 | 49.589 | 1.00 | 42.95  |
|    | ATOM | 1610 | N   | LEU | A | 209 | 14.623 | 59.350 | 48.773 | 1.00 | 40.92  |
|    | ATOM | 1611 | CA  | LEU | A | 209 | 15.739 | 58.440 | 48.825 | 1.00 | 39.55  |
|    | ATOM | 1612 | C   | LEU | A | 209 | 16.756 | 58.575 | 47.743 | 1.00 | 47.96  |
|    | ATOM | 1613 | O   | LEU | A | 209 | 16.420 | 58.843 | 46.597 | 1.00 | 49.44  |
| 25 | ATOM | 1614 | CB  | LEU | A | 209 | 15.269 | 56.994 | 48.894 | 1.00 | 37.97  |
|    | ATOM | 1615 | CG  | LEU | A | 209 | 14.420 | 56.803 | 50.129 | 1.00 | 40.46  |
|    | ATOM | 1616 | CD1 | LEU | A | 209 | 13.713 | 55.469 | 50.075 | 1.00 | 36.99  |
|    | ATOM | 1617 | CD2 | LEU | A | 209 | 15.283 | 56.921 | 51.387 | 1.00 | 43.31  |
|    | ATOM | 1618 | N   | GLU | A | 210 | 17.999 | 58.317 | 48.182 | 1.00 | 42.68  |
| 30 | ATOM | 1619 | CA  | GLU | A | 210 | 19.205 | 58.311 | 47.381 | 1.00 | 40.30  |
|    | ATOM | 1620 | C   | GLU | A | 210 | 19.965 | 57.056 | 47.693 | 1.00 | 47.51  |
|    | ATOM | 1621 | O   | GLU | A | 210 | 19.708 | 56.432 | 48.721 | 1.00 | 47.89  |
|    | ATOM | 1622 | CB  | GLU | A | 210 | 20.084 | 59.553 | 47.613 | 1.00 | 42.01  |
|    | ATOM | 1623 | CG  | GLU | A | 210 | 19.699 | 60.734 | 46.697 | 1.00 | 58.26  |
| 35 | ATOM | 1624 | CD  | GLU | A | 210 | 20.524 | 61.970 | 46.897 | 1.00 | 100.00 |
|    | ATOM | 1625 | OE1 | GLU | A | 210 | 21.629 | 61.968 | 47.451 | 1.00 | 95.26  |
|    | ATOM | 1626 | OE2 | GLU | A | 210 | 19.935 | 63.047 | 46.486 | 1.00 | 100.00 |
|    | ATOM | 1627 | N   | SER | A | 211 | 20.895 | 56.662 | 46.805 | 1.00 | 45.01  |
|    | ATOM | 1628 | CA  | SER | A | 211 | 21.661 | 55.442 | 47.013 | 1.00 | 42.25  |
| 40 | ATOM | 1629 | C   | SER | A | 211 | 23.143 | 55.535 | 46.667 | 1.00 | 43.37  |
|    | ATOM | 1630 | O   | SER | A | 211 | 23.649 | 56.493 | 46.086 | 1.00 | 46.43  |
|    | ATOM | 1631 | CB  | SER | A | 211 | 21.025 | 54.233 | 46.346 | 1.00 | 44.33  |
|    | ATOM | 1632 | OG  | SER | A | 211 | 21.274 | 54.244 | 44.934 | 1.00 | 54.15  |
|    | ATOM | 1633 | N   | ARG | A | 212 | 23.829 | 54.497 | 47.053 | 1.00 | 34.85  |
| 45 | ATOM | 1634 | CA  | ARG | A | 212 | 25.229 | 54.328 | 46.791 | 1.00 | 35.41  |
|    | ATOM | 1635 | C   | ARG | A | 212 | 25.430 | 52.838 | 46.567 | 1.00 | 45.39  |
|    | ATOM | 1636 | O   | ARG | A | 212 | 24.840 | 52.027 | 47.276 | 1.00 | 48.85  |
|    | ATOM | 1637 | CB  | ARG | A | 212 | 26.101 | 54.846 | 47.915 | 1.00 | 37.25  |
|    | ATOM | 1638 | CG  | ARG | A | 212 | 27.151 | 55.827 | 47.402 | 1.00 | 68.10  |
| 50 | ATOM | 1639 | CD  | ARG | A | 212 | 26.532 | 56.962 | 46.587 | 1.00 | 76.55  |
|    | ATOM | 1640 | NE  | ARG | A | 212 | 26.695 | 58.307 | 47.148 | 1.00 | 55.19  |
|    | ATOM | 1641 | CZ  | ARG | A | 212 | 25.845 | 59.301 | 46.867 | 1.00 | 70.87  |
|    | ATOM | 1642 | NH1 | ARG | A | 212 | 24.806 | 59.105 | 46.059 | 1.00 | 35.71  |
|    | ATOM | 1643 | NH2 | ARG | A | 212 | 26.032 | 60.516 | 47.392 | 1.00 | 73.35  |
| 55 | ATOM | 1644 | N   | GLN | A | 213 | 26.210 | 52.442 | 45.567 | 1.00 | 40.74  |
|    | ATOM | 1645 | CA  | GLN | A | 213 | 26.408 | 51.021 | 45.331 | 1.00 | 39.90  |
|    | ATOM | 1646 | C   | GLN | A | 213 | 27.646 | 50.537 | 46.050 | 1.00 | 46.34  |
|    | ATOM | 1647 | O   | GLN | A | 213 | 28.740 | 50.981 | 45.741 | 1.00 | 53.77  |
|    | ATOM | 1648 | CB  | GLN | A | 213 | 26.545 | 50.741 | 43.846 | 1.00 | 40.99  |
| 60 | ATOM | 1649 | CG  | GLN | A | 213 | 26.976 | 49.296 | 43.532 | 1.00 | 55.79  |
|    | ATOM | 1650 | CD  | GLN | A | 213 | 26.292 | 48.743 | 42.301 | 1.00 | 76.04  |
|    | ATOM | 1651 | OE1 | GLN | A | 213 | 26.275 | 47.523 | 42.102 | 1.00 | 86.66  |
|    | ATOM | 1652 | NE2 | GLN | A | 213 | 25.700 | 49.618 | 41.489 | 1.00 | 55.45  |
|    | ATOM | 1653 | N   | ILE | A | 214 | 27.495 | 49.649 | 47.013 | 1.00 | 33.12  |
|    | ATOM | 1654 | CA  | ILE | A | 214 | 28.663 | 49.206 | 47.743 | 1.00 | 32.55  |



|    |      |      |     |           |        |        |        |      |       |
|----|------|------|-----|-----------|--------|--------|--------|------|-------|
|    | ATOM | 1655 | C   | ILE A 214 | 28.911 | 47.765 | 47.536 | 1.00 | 39.29 |
|    | ATOM | 1656 | O   | ILE A 214 | 29.726 | 47.162 | 48.230 | 1.00 | 42.41 |
|    | ATOM | 1657 | CB  | ILE A 214 | 28.546 | 49.428 | 49.250 | 1.00 | 35.72 |
| 5  | ATOM | 1658 | CG1 | ILE A 214 | 27.395 | 48.573 | 49.791 | 1.00 | 36.13 |
|    | ATOM | 1659 | CG2 | ILE A 214 | 28.344 | 50.911 | 49.598 | 1.00 | 35.79 |
|    | ATOM | 1660 | CD1 | ILE A 214 | 27.067 | 48.841 | 51.260 | 1.00 | 46.69 |
|    | ATOM | 1661 | N   | GLY A 215 | 28.199 | 47.197 | 46.598 | 1.00 | 35.02 |
|    | ATOM | 1662 | CA  | GLY A 215 | 28.638 | 45.855 | 46.234 | 1.00 | 34.88 |
| 10 | ATOM | 1663 | C   | GLY A 215 | 27.970 | 45.405 | 44.950 | 1.00 | 41.09 |
|    | ATOM | 1664 | O   | GLY A 215 | 27.083 | 46.048 | 44.425 | 1.00 | 44.25 |
|    | ATOM | 1665 | N   | PRO A 216 | 28.448 | 44.262 | 44.410 | 1.00 | 39.62 |
|    | ATOM | 1666 | CA  | PRO A 216 | 27.890 | 43.720 | 43.197 | 1.00 | 39.69 |
|    | ATOM | 1667 | C   | PRO A 216 | 26.369 | 43.661 | 43.253 | 1.00 | 41.56 |
| 15 | ATOM | 1668 | O   | PRO A 216 | 25.655 | 43.817 | 42.240 | 1.00 | 44.35 |
|    | ATOM | 1669 | CB  | PRO A 216 | 28.448 | 42.311 | 42.996 | 1.00 | 39.91 |
|    | ATOM | 1670 | CG  | PRO A 216 | 29.377 | 41.993 | 44.164 | 1.00 | 41.54 |
|    | ATOM | 1671 | CD  | PRO A 216 | 29.514 | 43.411 | 44.897 | 1.00 | 37.70 |
|    | ATOM | 1672 | N   | ARG A 217 | 25.846 | 43.398 | 44.477 | 1.00 | 31.04 |
| 20 | ATOM | 1673 | CA  | ARG A 217 | 24.421 | 43.328 | 44.652 | 1.00 | 29.22 |
|    | ATOM | 1674 | C   | ARG A 217 | 23.928 | 44.109 | 45.872 | 1.00 | 38.24 |
|    | ATOM | 1675 | O   | ARG A 217 | 22.861 | 43.885 | 46.368 | 1.00 | 40.69 |
|    | ATOM | 1676 | CB  | ARG A 217 | 24.012 | 41.844 | 44.790 | 1.00 | 22.75 |
|    | ATOM | 1677 | CG  | ARG A 217 | 25.221 | 40.963 | 45.109 | 1.00 | 40.77 |
| 25 | ATOM | 1678 | CD  | ARG A 217 | 24.828 | 39.774 | 45.985 | 1.00 | 34.08 |
|    | ATOM | 1679 | NE  | ARG A 217 | 26.020 | 39.183 | 46.581 | 1.00 | 45.20 |
|    | ATOM | 1680 | CZ  | ARG A 217 | 25.955 | 37.894 | 46.911 | 1.00 | 65.13 |
|    | ATOM | 1681 | NH1 | ARG A 217 | 24.832 | 37.220 | 46.716 | 1.00 | 42.40 |
|    | ATOM | 1682 | NH2 | ARG A 217 | 26.997 | 37.300 | 47.472 | 1.00 | 48.08 |
| 30 | ATOM | 1683 | N   | THR A 218 | 24.784 | 45.022 | 46.404 | 1.00 | 31.00 |
|    | ATOM | 1684 | CA  | THR A 218 | 24.309 | 45.886 | 47.487 | 1.00 | 31.00 |
|    | ATOM | 1685 | C   | THR A 218 | 24.128 | 47.319 | 47.021 | 1.00 | 43.60 |
|    | ATOM | 1686 | O   | THR A 218 | 25.065 | 47.930 | 46.512 | 1.00 | 48.42 |
|    | ATOM | 1687 | CB  | THR A 218 | 25.315 | 45.845 | 48.640 | 1.00 | 36.95 |
| 35 | ATOM | 1688 | OG1 | THR A 218 | 25.430 | 44.517 | 49.139 | 1.00 | 45.66 |
|    | ATOM | 1689 | CG2 | THR A 218 | 24.826 | 46.751 | 49.766 | 1.00 | 34.17 |
|    | ATOM | 1690 | N   | LEU A 219 | 23.099 | 48.018 | 47.431 | 1.00 | 39.19 |
|    | ATOM | 1691 | CA  | LEU A 219 | 23.055 | 49.452 | 47.315 | 1.00 | 38.18 |
|    | ATOM | 1692 | C   | LEU A 219 | 22.713 | 50.000 | 48.695 | 1.00 | 42.32 |
| 40 | ATOM | 1693 | O   | LEU A 219 | 22.108 | 49.289 | 49.498 | 1.00 | 43.67 |
|    | ATOM | 1694 | CB  | LEU A 219 | 21.927 | 49.841 | 46.356 | 1.00 | 37.05 |
|    | ATOM | 1695 | CG  | LEU A 219 | 22.386 | 50.657 | 45.168 | 1.00 | 39.31 |
|    | ATOM | 1696 | CD1 | LEU A 219 | 23.670 | 50.064 | 44.613 | 1.00 | 40.57 |
|    | ATOM | 1697 | CD2 | LEU A 219 | 21.283 | 50.619 | 44.131 | 1.00 | 29.39 |
| 45 | ATOM | 1698 | N   | VAL A 220 | 23.066 | 51.241 | 48.976 | 1.00 | 35.01 |
|    | ATOM | 1699 | CA  | VAL A 220 | 22.741 | 51.830 | 50.253 | 1.00 | 36.98 |
|    | ATOM | 1700 | C   | VAL A 220 | 21.736 | 52.923 | 50.043 | 1.00 | 44.08 |
|    | ATOM | 1701 | O   | VAL A 220 | 21.959 | 53.835 | 49.256 | 1.00 | 46.60 |
|    | ATOM | 1702 | CB  | VAL A 220 | 23.965 | 52.346 | 51.028 | 1.00 | 44.95 |
| 50 | ATOM | 1703 | CG1 | VAL A 220 | 23.675 | 52.428 | 52.516 | 1.00 | 43.16 |
|    | ATOM | 1704 | CG2 | VAL A 220 | 25.138 | 51.382 | 50.828 | 1.00 | 47.70 |
|    | ATOM | 1705 | N   | TRP A 221 | 20.622 | 52.818 | 50.731 | 1.00 | 41.98 |
|    | ATOM | 1706 | CA  | TRP A 221 | 19.605 | 53.828 | 50.602 | 1.00 | 41.64 |
|    | ATOM | 1707 | C   | TRP A 221 | 19.464 | 54.612 | 51.872 | 1.00 | 42.40 |
| 55 | ATOM | 1708 | O   | TRP A 221 | 19.461 | 54.060 | 52.960 | 1.00 | 45.56 |
|    | ATOM | 1709 | CB  | TRP A 221 | 18.256 | 53.245 | 50.186 | 1.00 | 41.24 |
|    | ATOM | 1710 | CG  | TRP A 221 | 18.353 | 52.459 | 48.918 | 1.00 | 42.59 |
|    | ATOM | 1711 | CD1 | TRP A 221 | 18.888 | 51.225 | 48.793 | 1.00 | 45.35 |
|    | ATOM | 1712 | CD2 | TRP A 221 | 17.949 | 52.873 | 47.590 | 1.00 | 41.62 |
| 60 | ATOM | 1713 | NE1 | TRP A 221 | 18.826 | 50.832 | 47.478 | 1.00 | 44.74 |
|    | ATOM | 1714 | CE2 | TRP A 221 | 18.243 | 51.821 | 46.720 | 1.00 | 45.31 |
|    | ATOM | 1715 | CE3 | TRP A 221 | 17.345 | 54.009 | 47.061 | 1.00 | 41.17 |
|    | ATOM | 1716 | CZ2 | TRP A 221 | 17.958 | 51.902 | 45.346 | 1.00 | 42.60 |
|    | ATOM | 1717 | CZ3 | TRP A 221 | 17.054 | 54.083 | 45.710 | 1.00 | 39.08 |
|    | ATOM | 1718 | CH2 | TRP A 221 | 17.360 | 53.040 | 44.864 | 1.00 | 38.48 |



|    |      |      |     |           |        |        |        |      |        |
|----|------|------|-----|-----------|--------|--------|--------|------|--------|
|    | ATOM | 1719 | N   | SER A 222 | 19.271 | 55.896 | 51.688 | 1.00 | 37.01  |
|    | ATOM | 1720 | CA  | SER A 222 | 19.017 | 56.846 | 52.748 | 1.00 | 38.05  |
|    | ATOM | 1721 | C   | SER A 222 | 18.853 | 58.251 | 52.205 | 1.00 | 45.28  |
| 5  | ATOM | 1722 | O   | SER A 222 | 19.005 | 58.503 | 51.008 | 1.00 | 44.02  |
|    | ATOM | 1723 | CB  | SER A 222 | 20.098 | 56.816 | 53.820 | 1.00 | 39.07  |
|    | ATOM | 1724 | OG  | SER A 222 | 21.322 | 57.149 | 53.229 | 1.00 | 42.36  |
|    | ATOM | 1725 | N   | GLU A 223 | 18.586 | 59.190 | 53.088 | 1.00 | 40.91  |
|    | ATOM | 1726 | CA  | GLU A 223 | 18.465 | 60.527 | 52.584 | 1.00 | 41.97  |
| 10 | ATOM | 1727 | C   | GLU A 223 | 19.843 | 61.042 | 52.234 | 1.00 | 50.17  |
|    | ATOM | 1728 | O   | GLU A 223 | 20.829 | 60.701 | 52.863 | 1.00 | 52.02  |
|    | ATOM | 1729 | CB  | GLU A 223 | 17.856 | 61.483 | 53.597 | 1.00 | 43.06  |
|    | ATOM | 1730 | CG  | GLU A 223 | 16.364 | 61.262 | 53.861 | 1.00 | 51.71  |
|    | ATOM | 1731 | CD  | GLU A 223 | 15.799 | 62.478 | 54.545 | 1.00 | 84.51  |
|    | ATOM | 1732 | OE1 | GLU A 223 | 15.905 | 63.610 | 54.085 | 1.00 | 56.82  |
| 15 | ATOM | 1733 | OE2 | GLU A 223 | 15.244 | 62.222 | 55.705 | 1.00 | 88.87  |
|    | ATOM | 1734 | N   | LYS A 224 | 19.892 | 61.875 | 51.229 | 1.00 | 47.39  |
|    | ATOM | 1735 | CA  | LYS A 224 | 21.139 | 62.456 | 50.792 | 1.00 | 48.51  |
|    | ATOM | 1736 | C   | LYS A 224 | 22.163 | 62.683 | 51.930 | 1.00 | 50.90  |
|    | ATOM | 1737 | O   | LYS A 224 | 23.382 | 62.569 | 51.736 | 1.00 | 51.55  |
| 20 | ATOM | 1738 | CB  | LYS A 224 | 20.843 | 63.736 | 49.986 | 1.00 | 51.58  |
|    | ATOM | 1739 | CG  | LYS A 224 | 22.039 | 64.648 | 49.723 | 1.00 | 81.16  |
|    | ATOM | 1740 | CD  | LYS A 224 | 21.954 | 65.397 | 48.392 | 1.00 | 97.82  |
|    | ATOM | 1741 | CE  | LYS A 224 | 21.646 | 66.891 | 48.530 | 1.00 | 100.00 |
|    | ATOM | 1742 | NZ  | LYS A 224 | 22.056 | 67.700 | 47.362 | 1.00 | 100.00 |
| 25 | ATOM | 1743 | N   | GLU A 225 | 21.683 | 63.011 | 53.123 | 1.00 | 45.77  |
|    | ATOM | 1744 | CA  | GLU A 225 | 22.607 | 63.309 | 54.199 | 1.00 | 46.00  |
|    | ATOM | 1745 | C   | GLU A 225 | 23.227 | 62.150 | 54.902 | 1.00 | 47.99  |
|    | ATOM | 1746 | O   | GLU A 225 | 24.107 | 62.354 | 55.732 | 1.00 | 47.21  |
|    | ATOM | 1747 | CB  | GLU A 225 | 22.057 | 64.296 | 55.210 | 1.00 | 47.71  |
| 30 | ATOM | 1748 | CG  | GLU A 225 | 20.530 | 64.296 | 55.182 | 1.00 | 63.24  |
|    | ATOM | 1749 | CD  | GLU A 225 | 19.931 | 65.219 | 54.150 | 1.00 | 75.13  |
|    | ATOM | 1750 | OE1 | GLU A 225 | 20.187 | 66.420 | 54.046 | 1.00 | 54.64  |
|    | ATOM | 1751 | OE2 | GLU A 225 | 19.039 | 64.578 | 53.420 | 1.00 | 49.64  |
| 35 | ATOM | 1752 | N   | GLN A 226 | 22.798 | 60.949 | 54.564 | 1.00 | 43.92  |
|    | ATOM | 1753 | CA  | GLN A 226 | 23.340 | 59.772 | 55.224 | 1.00 | 43.91  |
|    | ATOM | 1754 | C   | GLN A 226 | 24.036 | 58.756 | 54.322 | 1.00 | 45.86  |
|    | ATOM | 1755 | O   | GLN A 226 | 24.756 | 57.871 | 54.806 | 1.00 | 45.70  |
|    | ATOM | 1756 | CB  | GLN A 226 | 22.252 | 59.084 | 56.063 | 1.00 | 45.27  |
|    | ATOM | 1757 | CG  | GLN A 226 | 21.965 | 59.790 | 57.400 | 1.00 | 31.17  |
| 40 | ATOM | 1758 | CD  | GLN A 226 | 21.297 | 61.155 | 57.302 | 1.00 | 44.48  |
|    | ATOM | 1759 | OE1 | GLN A 226 | 21.823 | 62.149 | 57.820 | 1.00 | 37.36  |
|    | ATOM | 1760 | NE2 | GLN A 226 | 20.115 | 61.202 | 56.696 | 1.00 | 30.28  |
|    | ATOM | 1761 | N   | VAL A 227 | 23.814 | 58.871 | 53.021 | 1.00 | 41.20  |
|    | ATOM | 1762 | CA  | VAL A 227 | 24.406 | 57.947 | 52.071 | 1.00 | 43.13  |
| 45 | ATOM | 1763 | C   | VAL A 227 | 25.884 | 57.670 | 52.261 | 1.00 | 50.55  |
|    | ATOM | 1764 | O   | VAL A 227 | 26.298 | 56.518 | 52.480 | 1.00 | 53.01  |
|    | ATOM | 1765 | CB  | VAL A 227 | 24.155 | 58.293 | 50.604 | 1.00 | 49.39  |
|    | ATOM | 1766 | CG1 | VAL A 227 | 24.319 | 57.029 | 49.771 | 1.00 | 48.89  |
|    | ATOM | 1767 | CG2 | VAL A 227 | 22.752 | 58.851 | 50.421 | 1.00 | 50.47  |
| 50 | ATOM | 1768 | N   | GLU A 228 | 26.696 | 58.718 | 52.170 | 1.00 | 44.08  |
|    | ATOM | 1769 | CA  | GLU A 228 | 28.123 | 58.542 | 52.310 | 1.00 | 41.71  |
|    | ATOM | 1770 | C   | GLU A 228 | 28.514 | 57.871 | 53.583 | 1.00 | 44.20  |
|    | ATOM | 1771 | O   | GLU A 228 | 29.227 | 56.868 | 53.589 | 1.00 | 44.88  |
|    | ATOM | 1772 | CB  | GLU A 228 | 28.935 | 59.824 | 52.102 | 1.00 | 43.08  |
| 55 | ATOM | 1773 | CG  | GLU A 228 | 29.153 | 60.161 | 50.611 | 1.00 | 64.74  |
|    | ATOM | 1774 | CD  | GLU A 228 | 29.114 | 58.965 | 49.701 | 1.00 | 84.29  |
|    | ATOM | 1775 | OE1 | GLU A 228 | 29.975 | 58.107 | 49.685 | 1.00 | 84.36  |
|    | ATOM | 1776 | OE2 | GLU A 228 | 28.064 | 58.951 | 48.917 | 1.00 | 73.81  |
|    | ATOM | 1777 | N   | LYS A 229 | 28.066 | 58.423 | 54.685 | 1.00 | 39.79  |
| 60 | ATOM | 1778 | CA  | LYS A 229 | 28.449 | 57.796 | 55.922 | 1.00 | 39.04  |
|    | ATOM | 1779 | C   | LYS A 229 | 27.949 | 56.375 | 55.930 | 1.00 | 40.38  |
|    | ATOM | 1780 | O   | LYS A 229 | 28.639 | 55.433 | 56.346 | 1.00 | 43.63  |
|    | ATOM | 1781 | CB  | LYS A 229 | 28.129 | 58.585 | 57.187 | 1.00 | 39.79  |
|    | ATOM | 1782 | CG  | LYS A 229 | 28.903 | 58.072 | 58.394 | 1.00 | 63.75  |



|    |      |      |     |     |   |     |        |        |        |      |        |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
|    | ATOM | 1783 | CD  | LYS | A | 229 | 28.498 | 58.763 | 59.685 | 1.00 | 77.46  |
|    | ATOM | 1784 | CE  | LYS | A | 229 | 29.677 | 59.084 | 60.593 | 1.00 | 94.73  |
|    | ATOM | 1785 | NZ  | LYS | A | 229 | 30.344 | 60.353 | 60.256 | 1.00 | 100.00 |
| 5  | ATOM | 1786 | N   | SER | A | 230 | 26.741 | 56.220 | 55.428 | 1.00 | 28.48  |
|    | ATOM | 1787 | CA  | SER | A | 230 | 26.174 | 54.891 | 55.377 | 1.00 | 25.93  |
|    | ATOM | 1788 | C   | SER | A | 230 | 27.089 | 53.988 | 54.587 | 1.00 | 30.26  |
|    | ATOM | 1789 | O   | SER | A | 230 | 27.469 | 52.855 | 54.955 | 1.00 | 28.48  |
|    | ATOM | 1790 | CB  | SER | A | 230 | 24.824 | 54.927 | 54.694 | 1.00 | 30.08  |
| 10 | ATOM | 1791 | OG  | SER | A | 230 | 23.822 | 55.293 | 55.605 | 1.00 | 41.60  |
|    | ATOM | 1792 | N   | ALA | A | 231 | 27.436 | 54.536 | 53.459 | 1.00 | 31.13  |
|    | ATOM | 1793 | CA  | ALA | A | 231 | 28.288 | 53.820 | 52.593 | 1.00 | 36.66  |
|    | ATOM | 1794 | C   | ALA | A | 231 | 29.597 | 53.383 | 53.270 | 1.00 | 47.68  |
|    | ATOM | 1795 | O   | ALA | A | 231 | 30.003 | 52.238 | 53.103 | 1.00 | 54.59  |
|    | ATOM | 1796 | CB  | ALA | A | 231 | 28.406 | 54.518 | 51.257 | 1.00 | 38.49  |
| 15 | ATOM | 1797 | N   | TYR | A | 232 | 30.256 | 54.246 | 54.060 | 1.00 | 40.77  |
|    | ATOM | 1798 | CA  | TYR | A | 232 | 31.500 | 53.830 | 54.730 | 1.00 | 38.40  |
|    | ATOM | 1799 | C   | TYR | A | 232 | 31.265 | 52.721 | 55.753 | 1.00 | 39.70  |
|    | ATOM | 1800 | O   | TYR | A | 232 | 32.041 | 51.772 | 55.862 | 1.00 | 36.46  |
| 20 | ATOM | 1801 | CB  | TYR | A | 232 | 32.311 | 54.981 | 55.414 | 1.00 | 38.27  |
|    | ATOM | 1802 | CG  | TYR | A | 232 | 33.497 | 54.525 | 56.303 | 1.00 | 42.36  |
|    | ATOM | 1803 | CD1 | TYR | A | 232 | 34.755 | 54.238 | 55.753 | 1.00 | 46.41  |
|    | ATOM | 1804 | CD2 | TYR | A | 232 | 33.373 | 54.394 | 57.691 | 1.00 | 40.99  |
|    | ATOM | 1805 | CE1 | TYR | A | 232 | 35.835 | 53.815 | 56.534 | 1.00 | 47.23  |
| 25 | ATOM | 1806 | CE2 | TYR | A | 232 | 34.441 | 53.979 | 58.496 | 1.00 | 40.10  |
|    | ATOM | 1807 | CZ  | TYR | A | 232 | 35.680 | 53.695 | 57.916 | 1.00 | 48.59  |
|    | ATOM | 1808 | OH  | TYR | A | 232 | 36.734 | 53.282 | 58.698 | 1.00 | 51.92  |
|    | ATOM | 1809 | N   | GLU | A | 233 | 30.191 | 52.883 | 56.519 | 1.00 | 35.75  |
|    | ATOM | 1810 | CA  | GLU | A | 233 | 29.835 | 51.984 | 57.606 | 1.00 | 34.55  |
| 30 | ATOM | 1811 | C   | GLU | A | 233 | 29.633 | 50.498 | 57.252 | 1.00 | 38.39  |
|    | ATOM | 1812 | O   | GLU | A | 233 | 30.152 | 49.576 | 57.892 | 1.00 | 38.55  |
|    | ATOM | 1813 | CB  | GLU | A | 233 | 28.673 | 52.623 | 58.414 | 1.00 | 34.48  |
|    | ATOM | 1814 | CG  | GLU | A | 233 | 28.666 | 52.262 | 59.912 | 1.00 | 24.95  |
|    | ATOM | 1815 | CD  | GLU | A | 233 | 29.463 | 53.183 | 60.787 | 1.00 | 37.55  |
| 35 | ATOM | 1816 | OE1 | GLU | A | 233 | 29.408 | 54.410 | 60.741 | 1.00 | 55.33  |
|    | ATOM | 1817 | OE2 | GLU | A | 233 | 30.216 | 52.518 | 61.619 | 1.00 | 40.65  |
|    | ATOM | 1818 | N   | PHE | A | 234 | 28.867 | 50.282 | 56.202 | 1.00 | 33.02  |
|    | ATOM | 1819 | CA  | PHE | A | 234 | 28.493 | 48.974 | 55.719 | 1.00 | 29.90  |
|    | ATOM | 1820 | C   | PHE | A | 234 | 29.341 | 48.398 | 54.592 | 1.00 | 34.69  |
| 40 | ATOM | 1821 | O   | PHE | A | 234 | 28.883 | 47.521 | 53.823 | 1.00 | 34.21  |
|    | ATOM | 1822 | CB  | PHE | A | 234 | 27.020 | 49.081 | 55.293 | 1.00 | 30.23  |
|    | ATOM | 1823 | CG  | PHE | A | 234 | 26.215 | 49.752 | 56.394 | 1.00 | 30.32  |
|    | ATOM | 1824 | CD1 | PHE | A | 234 | 26.518 | 49.521 | 57.739 | 1.00 | 31.50  |
|    | ATOM | 1825 | CD2 | PHE | A | 234 | 25.151 | 50.605 | 56.102 | 1.00 | 28.66  |
| 45 | ATOM | 1826 | CE1 | PHE | A | 234 | 25.780 | 50.103 | 58.772 | 1.00 | 30.43  |
|    | ATOM | 1827 | CE2 | PHE | A | 234 | 24.407 | 51.203 | 57.121 | 1.00 | 29.60  |
|    | ATOM | 1828 | CZ  | PHE | A | 234 | 24.725 | 50.959 | 58.458 | 1.00 | 27.47  |
|    | ATOM | 1829 | N   | SER | A | 235 | 30.571 | 48.874 | 54.476 | 1.00 | 29.55  |
|    | ATOM | 1830 | CA  | SER | A | 235 | 31.428 | 48.366 | 53.412 | 1.00 | 28.64  |
| 50 | ATOM | 1831 | C   | SER | A | 235 | 31.387 | 46.858 | 53.338 | 1.00 | 30.38  |
|    | ATOM | 1832 | O   | SER | A | 235 | 31.166 | 46.252 | 52.282 | 1.00 | 32.37  |
|    | ATOM | 1833 | CB  | SER | A | 235 | 32.861 | 48.787 | 53.604 | 1.00 | 31.15  |
|    | ATOM | 1834 | OG  | SER | A | 235 | 33.028 | 49.368 | 54.873 | 1.00 | 39.32  |
|    | ATOM | 1835 | N   | GLU | A | 236 | 31.698 | 46.299 | 54.504 | 1.00 | 22.49  |
| 55 | ATOM | 1836 | CA  | GLU | A | 236 | 31.815 | 44.873 | 54.737 | 1.00 | 23.79  |
|    | ATOM | 1837 | C   | GLU | A | 236 | 30.627 | 43.992 | 54.380 | 1.00 | 32.37  |
|    | ATOM | 1838 | O   | GLU | A | 236 | 30.697 | 42.772 | 54.545 | 1.00 | 29.91  |
|    | ATOM | 1839 | CB  | GLU | A | 236 | 32.305 | 44.529 | 56.134 | 1.00 | 24.06  |
|    | ATOM | 1840 | CG  | GLU | A | 236 | 33.491 | 45.403 | 56.585 | 1.00 | 22.96  |
| 60 | ATOM | 1841 | CD  | GLU | A | 236 | 33.600 | 45.492 | 58.090 | 1.00 | 66.18  |
|    | ATOM | 1842 | OE1 | GLU | A | 236 | 32.633 | 45.482 | 58.849 | 1.00 | 37.01  |
|    | ATOM | 1843 | OE2 | GLU | A | 236 | 34.848 | 45.518 | 58.494 | 1.00 | 78.68  |
|    | ATOM | 1844 | N   | THR | A | 237 | 29.560 | 44.593 | 53.891 | 1.00 | 34.11  |
|    | ATOM | 1845 | CA  | THR | A | 237 | 28.384 | 43.823 | 53.539 | 1.00 | 33.69  |
|    | ATOM | 1846 | C   | THR | A | 237 | 28.644 | 42.609 | 52.644 | 1.00 | 33.33  |



|    |      |      |     |     |   |     |        |        |        |      |        |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
|    | ATOM | 1847 | O   | THR | A | 237 | 28.517 | 41.451 | 53.048 | 1.00 | 31.09  |
|    | ATOM | 1848 | CB  | THR | A | 237 | 27.218 | 44.710 | 53.057 | 1.00 | 37.99  |
|    | ATOM | 1849 | OG1 | THR | A | 237 | 26.899 | 45.675 | 54.048 | 1.00 | 33.49  |
| 5  | ATOM | 1850 | CG2 | THR | A | 237 | 25.995 | 43.862 | 52.744 | 1.00 | 25.66  |
|    | ATOM | 1851 | N   | GLU | A | 238 | 29.020 | 42.854 | 51.409 | 1.00 | 29.69  |
|    | ATOM | 1852 | CA  | GLU | A | 238 | 29.267 | 41.734 | 50.520 | 1.00 | 27.05  |
|    | ATOM | 1853 | C   | GLU | A | 238 | 30.071 | 40.638 | 51.146 | 1.00 | 33.17  |
|    | ATOM | 1854 | O   | GLU | A | 238 | 29.660 | 39.497 | 51.055 | 1.00 | 38.50  |
| 10 | ATOM | 1855 | CB  | GLU | A | 238 | 29.851 | 42.080 | 49.161 | 1.00 | 27.50  |
|    | ATOM | 1856 | CG  | GLU | A | 238 | 30.116 | 40.813 | 48.320 | 1.00 | 18.83  |
|    | ATOM | 1857 | CD  | GLU | A | 238 | 28.902 | 40.297 | 47.596 | 1.00 | 41.67  |
|    | ATOM | 1858 | OE1 | GLU | A | 238 | 27.848 | 40.909 | 47.464 | 1.00 | 33.59  |
|    | ATOM | 1859 | OE2 | GLU | A | 238 | 29.085 | 39.089 | 47.138 | 1.00 | 46.30  |
| 15 | ATOM | 1860 | N   | SER | A | 239 | 31.203 | 40.973 | 51.772 | 1.00 | 24.44  |
|    | ATOM | 1861 | CA  | SER | A | 239 | 32.045 | 39.957 | 52.387 | 1.00 | 24.60  |
|    | ATOM | 1862 | C   | SER | A | 239 | 31.245 | 39.060 | 53.344 | 1.00 | 35.72  |
|    | ATOM | 1863 | O   | SER | A | 239 | 31.379 | 37.830 | 53.360 | 1.00 | 35.25  |
|    | ATOM | 1864 | CB  | SER | A | 239 | 33.231 | 40.601 | 53.074 | 1.00 | 29.14  |
| 20 | ATOM | 1865 | OG  | SER | A | 239 | 32.747 | 41.590 | 53.961 | 1.00 | 54.60  |
|    | ATOM | 1866 | N   | MET | A | 240 | 30.382 | 39.703 | 54.154 | 1.00 | 33.13  |
|    | ATOM | 1867 | CA  | MET | A | 240 | 29.529 | 38.993 | 55.091 | 1.00 | 28.55  |
|    | ATOM | 1868 | C   | MET | A | 240 | 28.603 | 38.075 | 54.325 | 1.00 | 35.65  |
|    | ATOM | 1869 | O   | MET | A | 240 | 28.435 | 36.926 | 54.689 | 1.00 | 35.99  |
| 25 | ATOM | 1870 | CB  | MET | A | 240 | 28.736 | 39.945 | 55.993 | 1.00 | 26.50  |
|    | ATOM | 1871 | CG  | MET | A | 240 | 29.691 | 40.675 | 56.910 | 1.00 | 27.57  |
|    | ATOM | 1872 | SD  | MET | A | 240 | 28.871 | 41.986 | 57.833 | 1.00 | 32.91  |
|    | ATOM | 1873 | CE  | MET | A | 240 | 30.040 | 42.085 | 59.183 | 1.00 | 28.47  |
|    | ATOM | 1874 | N   | LEU | A | 241 | 28.019 | 38.603 | 53.243 | 1.00 | 32.77  |
| 30 | ATOM | 1875 | CA  | LEU | A | 241 | 27.120 | 37.859 | 52.381 | 1.00 | 29.87  |
|    | ATOM | 1876 | C   | LEU | A | 241 | 27.848 | 36.615 | 51.878 | 1.00 | 36.76  |
|    | ATOM | 1877 | O   | LEU | A | 241 | 27.302 | 35.509 | 51.858 | 1.00 | 36.97  |
|    | ATOM | 1878 | CB  | LEU | A | 241 | 26.715 | 38.753 | 51.196 | 1.00 | 29.71  |
|    | ATOM | 1879 | CG  | LEU | A | 241 | 25.283 | 39.289 | 51.237 | 1.00 | 37.68  |
| 35 | ATOM | 1880 | CD1 | LEU | A | 241 | 25.174 | 40.552 | 50.389 | 1.00 | 35.76  |
|    | ATOM | 1881 | CD2 | LEU | A | 241 | 24.309 | 38.257 | 50.673 | 1.00 | 45.60  |
|    | ATOM | 1882 | N   | LYS | A | 242 | 29.114 | 36.806 | 51.468 | 1.00 | 34.76  |
|    | ATOM | 1883 | CA  | LYS | A | 242 | 29.908 | 35.702 | 50.972 | 1.00 | 33.62  |
|    | ATOM | 1884 | C   | LYS | A | 242 | 30.072 | 34.690 | 52.039 | 1.00 | 32.18  |
| 40 | ATOM | 1885 | O   | LYS | A | 242 | 29.887 | 33.512 | 51.795 | 1.00 | 32.56  |
|    | ATOM | 1886 | CB  | LYS | A | 242 | 31.292 | 36.069 | 50.468 | 1.00 | 38.43  |
|    | ATOM | 1887 | CG  | LYS | A | 242 | 31.406 | 36.263 | 48.961 | 1.00 | 49.23  |
|    | ATOM | 1888 | CD  | LYS | A | 242 | 31.160 | 37.721 | 48.536 | 1.00 | 88.36  |
|    | ATOM | 1889 | CE  | LYS | A | 242 | 32.371 | 38.456 | 47.943 | 1.00 | 100.00 |
| 45 | ATOM | 1890 | NZ  | LYS | A | 242 | 32.033 | 39.411 | 46.862 | 1.00 | 100.00 |
|    | ATOM | 1891 | N   | ILE | A | 243 | 30.428 | 35.154 | 53.227 | 1.00 | 30.87  |
|    | ATOM | 1892 | CA  | ILE | A | 243 | 30.627 | 34.229 | 54.359 | 1.00 | 31.70  |
|    | ATOM | 1893 | C   | ILE | A | 243 | 29.381 | 33.458 | 54.764 | 1.00 | 36.50  |
|    | ATOM | 1894 | O   | ILE | A | 243 | 29.458 | 32.303 | 55.119 | 1.00 | 39.33  |
| 50 | ATOM | 1895 | CB  | ILE | A | 243 | 31.227 | 34.886 | 55.579 | 1.00 | 32.36  |
|    | ATOM | 1896 | CG1 | ILE | A | 243 | 32.630 | 35.337 | 55.222 | 1.00 | 32.09  |
|    | ATOM | 1897 | CG2 | ILE | A | 243 | 31.243 | 33.891 | 56.718 | 1.00 | 28.26  |
|    | ATOM | 1898 | CD1 | ILE | A | 243 | 33.035 | 36.578 | 55.981 | 1.00 | 20.09  |
|    | ATOM | 1899 | N   | ALA | A | 244 | 28.237 | 34.120 | 54.708 | 1.00 | 32.10  |
| 55 | ATOM | 1900 | CA  | ALA | A | 244 | 26.968 | 33.519 | 55.066 | 1.00 | 32.95  |
|    | ATOM | 1901 | C   | ALA | A | 244 | 26.600 | 32.392 | 54.127 | 1.00 | 36.35  |
|    | ATOM | 1902 | O   | ALA | A | 244 | 26.074 | 31.358 | 54.546 | 1.00 | 36.88  |
|    | ATOM | 1903 | CB  | ALA | A | 244 | 25.858 | 34.576 | 55.123 | 1.00 | 34.02  |
|    | ATOM | 1904 | N   | GLU | A | 245 | 26.890 | 32.617 | 52.846 | 1.00 | 31.20  |
| 60 | ATOM | 1905 | CA  | GLU | A | 245 | 26.614 | 31.635 | 51.818 | 1.00 | 29.26  |
|    | ATOM | 1906 | C   | GLU | A | 245 | 27.360 | 30.354 | 52.092 | 1.00 | 35.18  |
|    | ATOM | 1907 | O   | GLU | A | 245 | 26.849 | 29.276 | 51.800 | 1.00 | 36.21  |
|    | ATOM | 1908 | CB  | GLU | A | 245 | 26.908 | 32.177 | 50.421 | 1.00 | 30.22  |
|    | ATOM | 1909 | CG  | GLU | A | 245 | 25.701 | 32.938 | 49.842 | 1.00 | 39.79  |
|    | ATOM | 1910 | CD  | GLU | A | 245 | 26.026 | 33.564 | 48.529 | 1.00 | 51.91  |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
|    | ATOM | 1911 | OE1 | GLU | A | 245 | 26.945 | 34.351 | 48.358 | 1.00 | 34.19 |
|    | ATOM | 1912 | OE2 | GLU | A | 245 | 25.246 | 33.142 | 47.585 | 1.00 | 47.48 |
|    | ATOM | 1913 | N   | ASP | A | 246 | 28.570 | 30.484 | 52.680 | 1.00 | 32.29 |
| 5  | ATOM | 1914 | CA  | ASP | A | 246 | 29.417 | 29.350 | 53.033 | 1.00 | 30.70 |
|    | ATOM | 1915 | C   | ASP | A | 246 | 28.848 | 28.645 | 54.230 | 1.00 | 35.47 |
|    | ATOM | 1916 | O   | ASP | A | 246 | 28.881 | 27.417 | 54.347 | 1.00 | 37.08 |
|    | ATOM | 1917 | CB  | ASP | A | 246 | 30.873 | 29.717 | 53.355 | 1.00 | 33.17 |
|    | ATOM | 1918 | CG  | ASP | A | 246 | 31.709 | 28.473 | 53.413 | 1.00 | 64.49 |
| 10 | ATOM | 1919 | OD1 | ASP | A | 246 | 31.934 | 27.789 | 52.437 | 1.00 | 67.15 |
|    | ATOM | 1920 | OD2 | ASP | A | 246 | 32.118 | 28.167 | 54.622 | 1.00 | 79.01 |
|    | ATOM | 1921 | N   | LEU | A | 247 | 28.323 | 29.434 | 55.134 | 1.00 | 33.59 |
|    | ATOM | 1922 | CA  | LEU | A | 247 | 27.731 | 28.868 | 56.334 | 1.00 | 36.70 |
|    | ATOM | 1923 | C   | LEU | A | 247 | 26.355 | 28.208 | 56.083 | 1.00 | 35.92 |
| 15 | ATOM | 1924 | O   | LEU | A | 247 | 26.060 | 27.110 | 56.551 | 1.00 | 30.77 |
|    | ATOM | 1925 | CB  | LEU | A | 247 | 27.562 | 29.954 | 57.435 | 1.00 | 38.34 |
|    | ATOM | 1926 | CG  | LEU | A | 247 | 28.732 | 30.100 | 58.394 | 1.00 | 44.30 |
|    | ATOM | 1927 | CD1 | LEU | A | 247 | 29.341 | 28.738 | 58.641 | 1.00 | 48.20 |
|    | ATOM | 1928 | CD2 | LEU | A | 247 | 29.779 | 31.013 | 57.815 | 1.00 | 35.25 |
| 20 | ATOM | 1929 | N   | GLY | A | 248 | 25.471 | 28.887 | 55.353 | 1.00 | 34.97 |
|    | ATOM | 1930 | CA  | GLY | A | 248 | 24.160 | 28.315 | 55.181 | 1.00 | 36.00 |
|    | ATOM | 1931 | C   | GLY | A | 248 | 23.754 | 27.976 | 53.778 | 1.00 | 37.99 |
|    | ATOM | 1932 | O   | GLY | A | 248 | 22.637 | 27.524 | 53.526 | 1.00 | 38.13 |
|    | ATOM | 1933 | N   | GLY | A | 249 | 24.637 | 28.158 | 52.849 | 1.00 | 30.74 |
| 25 | ATOM | 1934 | CA  | GLY | A | 249 | 24.203 | 27.852 | 51.526 | 1.00 | 30.15 |
|    | ATOM | 1935 | C   | GLY | A | 249 | 23.918 | 29.131 | 50.759 | 1.00 | 38.91 |
|    | ATOM | 1936 | O   | GLY | A | 249 | 24.126 | 30.240 | 51.238 | 1.00 | 41.32 |
|    | ATOM | 1937 | N   | PRO | A | 250 | 23.453 | 28.946 | 49.547 | 1.00 | 38.93 |
|    | ATOM | 1938 | CA  | PRO | A | 250 | 23.173 | 30.021 | 48.639 | 1.00 | 38.03 |
| 30 | ATOM | 1939 | C   | PRO | A | 250 | 22.203 | 31.078 | 49.096 | 1.00 | 42.17 |
|    | ATOM | 1940 | O   | PRO | A | 250 | 21.258 | 30.823 | 49.840 | 1.00 | 45.20 |
|    | ATOM | 1941 | CB  | PRO | A | 250 | 22.663 | 29.357 | 47.352 | 1.00 | 39.18 |
|    | ATOM | 1942 | CG  | PRO | A | 250 | 22.952 | 27.864 | 47.436 | 1.00 | 41.01 |
|    | ATOM | 1943 | CD  | PRO | A | 250 | 23.396 | 27.610 | 48.865 | 1.00 | 38.57 |
| 35 | ATOM | 1944 | N   | TYR | A | 251 | 22.486 | 32.275 | 48.600 | 1.00 | 35.37 |
|    | ATOM | 1945 | CA  | TYR | A | 251 | 21.692 | 33.461 | 48.817 | 1.00 | 34.87 |
|    | ATOM | 1946 | C   | TYR | A | 251 | 20.740 | 33.479 | 47.649 | 1.00 | 39.55 |
|    | ATOM | 1947 | O   | TYR | A | 251 | 21.125 | 33.794 | 46.535 | 1.00 | 42.57 |
|    | ATOM | 1948 | CB  | TYR | A | 251 | 22.540 | 34.759 | 48.790 | 1.00 | 35.07 |
| 40 | ATOM | 1949 | CG  | TYR | A | 251 | 21.711 | 35.980 | 49.119 | 1.00 | 35.25 |
|    | ATOM | 1950 | CD1 | TYR | A | 251 | 21.341 | 36.229 | 50.441 | 1.00 | 33.14 |
|    | ATOM | 1951 | CD2 | TYR | A | 251 | 21.260 | 36.846 | 48.121 | 1.00 | 37.98 |
|    | ATOM | 1952 | CE1 | TYR | A | 251 | 20.575 | 37.341 | 50.781 | 1.00 | 28.05 |
|    | ATOM | 1953 | CE2 | TYR | A | 251 | 20.492 | 37.967 | 48.443 | 1.00 | 40.05 |
| 45 | ATOM | 1954 | CZ  | TYR | A | 251 | 20.160 | 38.213 | 49.777 | 1.00 | 42.84 |
|    | ATOM | 1955 | OH  | TYR | A | 251 | 19.409 | 39.307 | 50.112 | 1.00 | 39.70 |
|    | ATOM | 1956 | N   | VAL | A | 252 | 19.510 | 33.102 | 47.914 | 1.00 | 32.21 |
|    | ATOM | 1957 | CA  | VAL | A | 252 | 18.495 | 33.003 | 46.899 | 1.00 | 30.05 |
|    | ATOM | 1958 | C   | VAL | A | 252 | 17.708 | 34.279 | 46.631 | 1.00 | 38.47 |
| 50 | ATOM | 1959 | O   | VAL | A | 252 | 17.000 | 34.340 | 45.640 | 1.00 | 40.65 |
|    | ATOM | 1960 | CB  | VAL | A | 252 | 17.560 | 31.845 | 47.253 | 1.00 | 31.27 |
|    | ATOM | 1961 | CG1 | VAL | A | 252 | 18.378 | 30.605 | 47.643 | 1.00 | 28.15 |
|    | ATOM | 1962 | CG2 | VAL | A | 252 | 16.614 | 32.234 | 48.405 | 1.00 | 30.93 |
|    | ATOM | 1963 | N   | TRP | A | 253 | 17.800 | 35.292 | 47.504 | 1.00 | 32.44 |
| 55 | ATOM | 1964 | CA  | TRP | A | 253 | 17.041 | 36.509 | 47.309 | 1.00 | 30.93 |
|    | ATOM | 1965 | C   | TRP | A | 253 | 17.468 | 37.341 | 46.119 | 1.00 | 43.56 |
|    | ATOM | 1966 | O   | TRP | A | 253 | 16.690 | 38.119 | 45.568 | 1.00 | 46.70 |
|    | ATOM | 1967 | CB  | TRP | A | 253 | 16.898 | 37.302 | 48.606 | 1.00 | 29.65 |
|    | ATOM | 1968 | CG  | TRP | A | 253 | 16.364 | 36.369 | 49.625 | 1.00 | 30.19 |
| 60 | ATOM | 1969 | CD1 | TRP | A | 253 | 17.086 | 35.546 | 50.413 | 1.00 | 32.81 |
|    | ATOM | 1970 | CD2 | TRP | A | 253 | 14.989 | 36.110 | 49.913 | 1.00 | 29.63 |
|    | ATOM | 1971 | NE1 | TRP | A | 253 | 16.251 | 34.794 | 51.194 | 1.00 | 30.69 |
|    | ATOM | 1972 | CE2 | TRP | A | 253 | 14.955 | 35.128 | 50.912 | 1.00 | 31.50 |
|    | ATOM | 1973 | CE3 | TRP | A | 253 | 13.789 | 36.637 | 49.450 | 1.00 | 30.18 |
|    | ATOM | 1974 | CZ2 | TRP | A | 253 | 13.746 | 34.657 | 51.433 | 1.00 | 30.31 |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
|    | ATOM | 1975 | CZ3 | TRP | A | 253 | 12.600 | 36.164 | 49.958 | 1.00 | 31.14 |
|    | ATOM | 1976 | CH2 | TRP | A | 253 | 12.579 | 35.176 | 50.946 | 1.00 | 31.37 |
|    | ATOM | 1977 | N   | GLY | A | 254 | 18.697 | 37.182 | 45.675 | 1.00 | 42.35 |
| 5  | ATOM | 1978 | CA  | GLY | A | 254 | 19.101 | 37.944 | 44.509 | 1.00 | 41.34 |
|    | ATOM | 1979 | C   | GLY | A | 254 | 19.875 | 39.192 | 44.858 | 1.00 | 45.47 |
|    | ATOM | 1980 | O   | GLY | A | 254 | 21.079 | 39.236 | 44.671 | 1.00 | 45.89 |
|    | ATOM | 1981 | N   | GLN | A | 255 | 19.160 | 40.210 | 45.351 | 1.00 | 41.86 |
|    | ATOM | 1982 | CA  | GLN | A | 255 | 19.746 | 41.488 | 45.675 | 1.00 | 38.67 |
| 10 | ATOM | 1983 | C   | GLN | A | 255 | 19.576 | 41.776 | 47.153 | 1.00 | 40.18 |
|    | ATOM | 1984 | O   | GLN | A | 255 | 18.494 | 41.811 | 47.659 | 1.00 | 38.67 |
|    | ATOM | 1985 | CB  | GLN | A | 255 | 19.023 | 42.552 | 44.836 | 1.00 | 37.82 |
|    | ATOM | 1986 | CG  | GLN | A | 255 | 19.455 | 43.979 | 45.169 | 1.00 | 50.17 |
|    | ATOM | 1987 | CD  | GLN | A | 255 | 20.618 | 44.368 | 44.283 | 1.00 | 62.88 |
| 15 | ATOM | 1988 | OE1 | GLN | A | 255 | 21.104 | 43.612 | 43.463 | 1.00 | 55.76 |
|    | ATOM | 1989 | NE2 | GLN | A | 255 | 21.057 | 45.625 | 44.479 | 1.00 | 34.97 |
|    | ATOM | 1990 | N   | TYR | A | 256 | 20.716 | 41.900 | 47.866 | 1.00 | 33.01 |
|    | ATOM | 1991 | CA  | TYR | A | 256 | 20.651 | 42.361 | 49.258 | 1.00 | 28.69 |
|    | ATOM | 1992 | C   | TYR | A | 256 | 20.891 | 43.854 | 49.329 | 1.00 | 26.72 |
| 20 | ATOM | 1993 | O   | TYR | A | 256 | 21.963 | 44.321 | 49.225 | 1.00 | 24.22 |
|    | ATOM | 1994 | CB  | TYR | A | 256 | 21.743 | 41.629 | 50.075 | 1.00 | 29.99 |
|    | ATOM | 1995 | CG  | TYR | A | 256 | 21.567 | 41.867 | 51.556 | 1.00 | 35.47 |
|    | ATOM | 1996 | CD1 | TYR | A | 256 | 20.582 | 41.200 | 52.250 | 1.00 | 35.76 |
|    | ATOM | 1997 | CD2 | TYR | A | 256 | 22.405 | 42.746 | 52.239 | 1.00 | 37.52 |
| 25 | ATOM | 1998 | CE1 | TYR | A | 256 | 20.436 | 41.396 | 53.599 | 1.00 | 25.80 |
|    | ATOM | 1999 | CE2 | TYR | A | 256 | 22.255 | 42.946 | 53.588 | 1.00 | 39.10 |
|    | ATOM | 2000 | CZ  | TYR | A | 256 | 21.283 | 42.275 | 54.268 | 1.00 | 31.78 |
|    | ATOM | 2001 | OH  | TYR | A | 256 | 21.153 | 42.433 | 55.631 | 1.00 | 37.35 |
|    | ATOM | 2002 | N   | ASP | A | 257 | 19.834 | 44.613 | 49.463 | 1.00 | 23.26 |
| 30 | ATOM | 2003 | CA  | ASP | A | 257 | 20.077 | 46.027 | 49.621 | 1.00 | 23.47 |
|    | ATOM | 2004 | C   | ASP | A | 257 | 19.977 | 46.444 | 51.071 | 1.00 | 35.90 |
|    | ATOM | 2005 | O   | ASP | A | 257 | 19.729 | 45.661 | 51.967 | 1.00 | 39.48 |
|    | ATOM | 2006 | CB  | ASP | A | 257 | 19.073 | 46.803 | 48.758 | 1.00 | 24.13 |
|    | ATOM | 2007 | CG  | ASP | A | 257 | 19.689 | 47.030 | 47.388 | 1.00 | 38.50 |
| 35 | ATOM | 2008 | OD1 | ASP | A | 257 | 20.843 | 46.675 | 47.220 | 1.00 | 42.61 |
|    | ATOM | 2009 | OD2 | ASP | A | 257 | 19.020 | 47.555 | 46.517 | 1.00 | 29.02 |
|    | ATOM | 2010 | N   | LEU | A | 258 | 20.370 | 47.661 | 51.386 | 1.00 | 30.86 |
|    | ATOM | 2011 | CA  | LEU | A | 258 | 20.306 | 48.159 | 52.735 | 1.00 | 27.50 |
|    | ATOM | 2012 | C   | LEU | A | 258 | 19.526 | 49.466 | 52.765 | 1.00 | 36.37 |
| 40 | ATOM | 2013 | O   | LEU | A | 258 | 19.620 | 50.302 | 51.840 | 1.00 | 37.98 |
|    | ATOM | 2014 | CB  | LEU | A | 258 | 21.727 | 48.442 | 53.274 | 1.00 | 24.71 |
|    | ATOM | 2015 | CG  | LEU | A | 258 | 22.552 | 47.191 | 53.491 | 1.00 | 31.13 |
|    | ATOM | 2016 | CD1 | LEU | A | 258 | 23.913 | 47.567 | 54.043 | 1.00 | 30.89 |
|    | ATOM | 2017 | CD2 | LEU | A | 258 | 21.854 | 46.282 | 54.500 | 1.00 | 33.65 |
| 45 | ATOM | 2018 | N   | LEU | A | 259 | 18.762 | 49.632 | 53.838 | 1.00 | 29.87 |
|    | ATOM | 2019 | CA  | LEU | A | 259 | 18.006 | 50.849 | 54.052 | 1.00 | 28.43 |
|    | ATOM | 2020 | C   | LEU | A | 259 | 18.283 | 51.453 | 55.446 | 1.00 | 31.30 |
|    | ATOM | 2021 | O   | LEU | A | 259 | 18.055 | 50.819 | 56.477 | 1.00 | 31.19 |
|    | ATOM | 2022 | CB  | LEU | A | 259 | 16.500 | 50.809 | 53.693 | 1.00 | 27.63 |
| 50 | ATOM | 2023 | CG  | LEU | A | 259 | 15.706 | 51.980 | 54.298 | 1.00 | 31.51 |
|    | ATOM | 2024 | CD1 | LEU | A | 259 | 16.026 | 53.300 | 53.605 | 1.00 | 32.32 |
|    | ATOM | 2025 | CD2 | LEU | A | 259 | 14.212 | 51.731 | 54.253 | 1.00 | 26.87 |
|    | ATOM | 2026 | N   | VAL | A | 260 | 18.807 | 52.683 | 55.447 | 1.00 | 25.88 |
|    | ATOM | 2027 | CA  | VAL | A | 260 | 19.105 | 53.435 | 56.638 | 1.00 | 25.99 |
| 55 | ATOM | 2028 | C   | VAL | A | 260 | 17.896 | 54.336 | 56.796 | 1.00 | 34.83 |
|    | ATOM | 2029 | O   | VAL | A | 260 | 17.647 | 55.187 | 55.959 | 1.00 | 41.92 |
|    | ATOM | 2030 | CB  | VAL | A | 260 | 20.390 | 54.234 | 56.408 | 1.00 | 29.97 |
|    | ATOM | 2031 | CG1 | VAL | A | 260 | 20.701 | 55.179 | 57.592 | 1.00 | 32.08 |
|    | ATOM | 2032 | CG2 | VAL | A | 260 | 21.563 | 53.295 | 56.130 | 1.00 | 26.15 |
| 60 | ATOM | 2033 | N   | LEU | A | 261 | 17.098 | 54.120 | 57.815 | 1.00 | 28.41 |
|    | ATOM | 2034 | CA  | LEU | A | 261 | 15.865 | 54.878 | 58.024 | 1.00 | 25.52 |
|    | ATOM | 2035 | C   | LEU | A | 261 | 16.016 | 56.054 | 58.948 | 1.00 | 29.42 |
|    | ATOM | 2036 | O   | LEU | A | 261 | 17.090 | 56.300 | 59.489 | 1.00 | 29.96 |
|    | ATOM | 2037 | CB  | LEU | A | 261 | 14.874 | 53.921 | 58.706 | 1.00 | 25.70 |
|    | ATOM | 2038 | CG  | LEU | A | 261 | 14.387 | 52.877 | 57.740 | 1.00 | 33.14 |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
|    | ATOM | 2039 | CD1 | LEU | A | 261 | 15.161 | 51.571 | 57.929 | 1.00 | 32.73 |
|    | ATOM | 2040 | CD2 | LEU | A | 261 | 12.900 | 52.686 | 57.935 | 1.00 | 43.74 |
|    | ATOM | 2041 | N   | PRO | A | 262 | 14.903 | 56.758 | 59.142 | 1.00 | 28.52 |
| 5  | ATOM | 2042 | CA  | PRO | A | 262 | 14.894 | 57.870 | 60.047 | 1.00 | 28.50 |
|    | ATOM | 2043 | C   | PRO | A | 262 | 15.152 | 57.294 | 61.432 | 1.00 | 35.36 |
|    | ATOM | 2044 | O   | PRO | A | 262 | 14.866 | 56.124 | 61.683 | 1.00 | 34.52 |
|    | ATOM | 2045 | CB  | PRO | A | 262 | 13.512 | 58.512 | 59.971 | 1.00 | 29.19 |
|    | ATOM | 2046 | CG  | PRO | A | 262 | 12.707 | 57.719 | 58.964 | 1.00 | 34.34 |
| 10 | ATOM | 2047 | CD  | PRO | A | 262 | 13.581 | 56.575 | 58.492 | 1.00 | 30.63 |
|    | ATOM | 2048 | N   | PRO | A | 263 | 15.706 | 58.105 | 62.327 | 1.00 | 31.50 |
|    | ATOM | 2049 | CA  | PRO | A | 263 | 16.060 | 57.657 | 63.673 | 1.00 | 28.77 |
|    | ATOM | 2050 | C   | PRO | A | 263 | 14.966 | 57.021 | 64.493 | 1.00 | 29.15 |
|    | ATOM | 2051 | O   | PRO | A | 263 | 15.256 | 56.335 | 65.434 | 1.00 | 26.36 |
| 15 | ATOM | 2052 | CB  | PRO | A | 263 | 16.652 | 58.867 | 64.392 | 1.00 | 29.16 |
|    | ATOM | 2053 | CG  | PRO | A | 263 | 16.851 | 59.954 | 63.335 | 1.00 | 31.55 |
|    | ATOM | 2054 | CD  | PRO | A | 263 | 15.994 | 59.558 | 62.138 | 1.00 | 29.17 |
|    | ATOM | 2055 | N   | SER | A | 264 | 13.712 | 57.258 | 64.143 | 1.00 | 33.87 |
|    | ATOM | 2056 | CA  | SER | A | 264 | 12.578 | 56.703 | 64.864 | 1.00 | 33.81 |
| 20 | ATOM | 2057 | C   | SER | A | 264 | 12.403 | 55.223 | 64.604 | 1.00 | 37.36 |
|    | ATOM | 2058 | O   | SER | A | 264 | 11.529 | 54.570 | 65.201 | 1.00 | 39.61 |
|    | ATOM | 2059 | CB  | SER | A | 264 | 11.280 | 57.423 | 64.576 | 1.00 | 35.61 |
|    | ATOM | 2060 | OG  | SER | A | 264 | 10.955 | 57.276 | 63.201 | 1.00 | 53.45 |
|    | ATOM | 2061 | N   | PHE | A | 265 | 13.213 | 54.684 | 63.710 | 1.00 | 29.00 |
| 25 | ATOM | 2062 | CA  | PHE | A | 265 | 13.136 | 53.256 | 63.453 | 1.00 | 28.56 |
|    | ATOM | 2063 | C   | PHE | A | 265 | 13.260 | 52.491 | 64.787 | 1.00 | 28.49 |
|    | ATOM | 2064 | O   | PHE | A | 265 | 14.208 | 52.675 | 65.533 | 1.00 | 27.36 |
|    | ATOM | 2065 | CB  | PHE | A | 265 | 14.200 | 52.833 | 62.454 | 1.00 | 31.40 |
|    | ATOM | 2066 | CG  | PHE | A | 265 | 13.875 | 51.458 | 62.028 | 1.00 | 34.51 |
| 30 | ATOM | 2067 | CD1 | PHE | A | 265 | 12.601 | 51.174 | 61.543 | 1.00 | 35.11 |
|    | ATOM | 2068 | CD2 | PHE | A | 265 | 14.814 | 50.435 | 62.156 | 1.00 | 38.94 |
|    | ATOM | 2069 | CE1 | PHE | A | 265 | 12.282 | 49.876 | 61.154 | 1.00 | 37.42 |
|    | ATOM | 2070 | CE2 | PHE | A | 265 | 14.511 | 49.131 | 61.772 | 1.00 | 42.65 |
|    | ATOM | 2071 | CZ  | PHE | A | 265 | 13.236 | 48.860 | 61.274 | 1.00 | 40.14 |
| 35 | ATOM | 2072 | N   | PRO | A | 266 | 12.272 | 51.650 | 65.128 | 1.00 | 24.06 |
|    | ATOM | 2073 | CA  | PRO | A | 266 | 12.249 | 50.945 | 66.419 | 1.00 | 20.62 |
|    | ATOM | 2074 | C   | PRO | A | 266 | 13.231 | 49.794 | 66.701 | 1.00 | 29.34 |
|    | ATOM | 2075 | O   | PRO | A | 266 | 13.343 | 49.364 | 67.847 | 1.00 | 28.17 |
|    | ATOM | 2076 | CB  | PRO | A | 266 | 10.808 | 50.463 | 66.593 | 1.00 | 19.16 |
| 40 | ATOM | 2077 | CG  | PRO | A | 266 | 10.076 | 50.686 | 65.281 | 1.00 | 21.07 |
|    | ATOM | 2078 | CD  | PRO | A | 266 | 11.046 | 51.355 | 64.325 | 1.00 | 19.44 |
|    | ATOM | 2079 | N   | TYR | A | 267 | 13.922 | 49.280 | 65.676 | 1.00 | 27.23 |
|    | ATOM | 2080 | CA  | TYR | A | 267 | 14.849 | 48.160 | 65.817 | 1.00 | 25.74 |
|    | ATOM | 2081 | C   | TYR | A | 267 | 16.181 | 48.454 | 65.189 | 1.00 | 32.57 |
| 45 | ATOM | 2082 | O   | TYR | A | 267 | 16.281 | 49.316 | 64.324 | 1.00 | 32.48 |
|    | ATOM | 2083 | CB  | TYR | A | 267 | 14.298 | 46.903 | 65.121 | 1.00 | 25.07 |
|    | ATOM | 2084 | CG  | TYR | A | 267 | 12.968 | 46.502 | 65.674 | 1.00 | 24.45 |
|    | ATOM | 2085 | CD1 | TYR | A | 267 | 12.915 | 45.765 | 66.856 | 1.00 | 27.05 |
|    | ATOM | 2086 | CD2 | TYR | A | 267 | 11.776 | 46.851 | 65.037 | 1.00 | 22.15 |
| 50 | ATOM | 2087 | CE1 | TYR | A | 267 | 11.697 | 45.387 | 67.419 | 1.00 | 25.01 |
|    | ATOM | 2088 | CE2 | TYR | A | 267 | 10.548 | 46.496 | 65.596 | 1.00 | 19.09 |
|    | ATOM | 2089 | CZ  | TYR | A | 267 | 10.510 | 45.767 | 66.786 | 1.00 | 17.98 |
|    | ATOM | 2090 | OH  | TYR | A | 267 | 9.302  | 45.416 | 67.353 | 1.00 | 19.51 |
|    | ATOM | 2091 | N   | GLY | A | 268 | 17.196 | 47.698 | 65.627 | 1.00 | 30.22 |
| 55 | ATOM | 2092 | CA  | GLY | A | 268 | 18.547 | 47.826 | 65.114 | 1.00 | 27.29 |
|    | ATOM | 2093 | C   | GLY | A | 268 | 18.485 | 47.620 | 63.614 | 1.00 | 29.82 |
|    | ATOM | 2094 | O   | GLY | A | 268 | 19.136 | 48.297 | 62.836 | 1.00 | 32.99 |
|    | ATOM | 2095 | N   | GLY | A | 269 | 17.637 | 46.676 | 63.228 | 1.00 | 23.19 |
|    | ATOM | 2096 | CA  | GLY | A | 269 | 17.393 | 46.320 | 61.853 | 1.00 | 21.62 |
| 60 | ATOM | 2097 | C   | GLY | A | 269 | 16.187 | 45.402 | 61.777 | 1.00 | 27.53 |
|    | ATOM | 2098 | O   | GLY | A | 269 | 15.681 | 44.948 | 62.820 | 1.00 | 20.14 |
|    | ATOM | 2099 | N   | MET | A | 270 | 15.735 | 45.154 | 60.528 | 1.00 | 27.81 |
|    | ATOM | 2100 | CA  | MET | A | 270 | 14.615 | 44.267 | 60.176 | 1.00 | 25.61 |
|    | ATOM | 2101 | C   | MET | A | 270 | 14.956 | 43.585 | 58.874 | 1.00 | 33.56 |
|    | ATOM | 2102 | O   | MET | A | 270 | 15.221 | 44.247 | 57.867 | 1.00 | 34.67 |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
|    | ATOM | 2103 | CB  | MET | A | 270 | 13.247 | 44.936 | 60.028 | 1.00 | 26.07 |
|    | ATOM | 2104 | CG  | MET | A | 270 | 12.195 | 43.937 | 59.602 | 1.00 | 28.81 |
|    | ATOM | 2105 | SD  | MET | A | 270 | 11.875 | 42.742 | 60.929 | 1.00 | 37.39 |
| 5  | ATOM | 2106 | CE  | MET | A | 270 | 10.720 | 41.621 | 60.082 | 1.00 | 35.30 |
|    | ATOM | 2107 | N   | GLU | A | 271 | 14.995 | 42.263 | 58.904 | 1.00 | 32.20 |
|    | ATOM | 2108 | CA  | GLU | A | 271 | 15.393 | 41.459 | 57.753 | 1.00 | 33.32 |
|    | ATOM | 2109 | C   | GLU | A | 271 | 14.419 | 41.382 | 56.567 | 1.00 | 40.86 |
|    | ATOM | 2110 | O   | GLU | A | 271 | 14.087 | 40.285 | 56.107 | 1.00 | 42.02 |
| 10 | ATOM | 2111 | CB  | GLU | A | 271 | 15.802 | 40.054 | 58.230 | 1.00 | 35.05 |
|    | ATOM | 2112 | CG  | GLU | A | 271 | 14.607 | 39.218 | 58.760 | 1.00 | 33.55 |
|    | ATOM | 2113 | CD  | GLU | A | 271 | 14.291 | 39.428 | 60.219 | 1.00 | 25.52 |
|    | ATOM | 2114 | OE1 | GLU | A | 271 | 14.586 | 40.436 | 60.844 | 1.00 | 37.23 |
|    | ATOM | 2115 | OE2 | GLU | A | 271 | 13.699 | 38.393 | 60.757 | 1.00 | 25.86 |
| 15 | ATOM | 2116 | N   | ASN | A | 272 | 13.978 | 42.535 | 56.052 | 1.00 | 35.34 |
|    | ATOM | 2117 | CA  | ASN | A | 272 | 13.057 | 42.544 | 54.928 | 1.00 | 33.26 |
|    | ATOM | 2118 | C   | ASN | A | 272 | 13.787 | 42.048 | 53.702 | 1.00 | 34.47 |
|    | ATOM | 2119 | O   | ASN | A | 272 | 14.811 | 42.613 | 53.351 | 1.00 | 33.64 |
|    | ATOM | 2120 | CB  | ASN | A | 272 | 12.441 | 43.947 | 54.719 | 1.00 | 30.65 |
| 20 | ATOM | 2121 | CG  | ASN | A | 272 | 11.667 | 44.453 | 55.935 | 1.00 | 42.50 |
|    | ATOM | 2122 | OD1 | ASN | A | 272 | 11.908 | 45.554 | 56.475 | 1.00 | 47.09 |
|    | ATOM | 2123 | ND2 | ASN | A | 272 | 10.716 | 43.661 | 56.371 | 1.00 | 24.31 |
|    | ATOM | 2124 | N   | PRO | A | 273 | 13.281 | 40.983 | 53.078 | 1.00 | 29.63 |
|    | ATOM | 2125 | CA  | PRO | A | 273 | 13.935 | 40.373 | 51.910 | 1.00 | 28.47 |
| 25 | ATOM | 2126 | C   | PRO | A | 273 | 14.303 | 41.345 | 50.819 | 1.00 | 30.43 |
|    | ATOM | 2127 | O   | PRO | A | 273 | 13.457 | 42.089 | 50.372 | 1.00 | 31.65 |
|    | ATOM | 2128 | CB  | PRO | A | 273 | 12.991 | 39.305 | 51.381 | 1.00 | 30.16 |
|    | ATOM | 2129 | CG  | PRO | A | 273 | 11.829 | 39.237 | 52.365 | 1.00 | 36.65 |
|    | ATOM | 2130 | CD  | PRO | A | 273 | 11.927 | 40.440 | 53.310 | 1.00 | 30.84 |
| 30 | ATOM | 2131 | N   | CYS | A | 274 | 15.571 | 41.333 | 50.431 | 1.00 | 27.40 |
|    | ATOM | 2132 | CA  | CYS | A | 274 | 16.069 | 42.206 | 49.373 | 1.00 | 28.17 |
|    | ATOM | 2133 | C   | CYS | A | 274 | 16.327 | 43.604 | 49.860 | 1.00 | 27.35 |
|    | ATOM | 2134 | O   | CYS | A | 274 | 17.114 | 44.345 | 49.248 | 1.00 | 28.53 |
|    | ATOM | 2135 | CB  | CYS | A | 274 | 15.121 | 42.347 | 48.145 | 1.00 | 32.00 |
| 35 | ATOM | 2136 | SG  | CYS | A | 274 | 14.659 | 40.798 | 47.340 | 1.00 | 38.42 |
|    | ATOM | 2137 | N   | LEU | A | 275 | 15.658 | 43.972 | 50.947 | 1.00 | 26.20 |
|    | ATOM | 2138 | CA  | LEU | A | 275 | 15.789 | 45.315 | 51.535 | 1.00 | 29.54 |
|    | ATOM | 2139 | C   | LEU | A | 275 | 15.857 | 45.279 | 53.059 | 1.00 | 32.52 |
|    | ATOM | 2140 | O   | LEU | A | 275 | 14.859 | 45.250 | 53.772 | 1.00 | 32.44 |
| 40 | ATOM | 2141 | CB  | LEU | A | 275 | 14.657 | 46.253 | 51.005 | 1.00 | 28.58 |
|    | ATOM | 2142 | CG  | LEU | A | 275 | 14.847 | 47.735 | 51.239 | 1.00 | 26.78 |
|    | ATOM | 2143 | CD1 | LEU | A | 275 | 16.191 | 48.183 | 50.698 | 1.00 | 21.90 |
|    | ATOM | 2144 | CD2 | LEU | A | 275 | 13.712 | 48.478 | 50.554 | 1.00 | 31.48 |
|    | ATOM | 2145 | N   | THR | A | 276 | 17.062 | 45.244 | 53.570 | 1.00 | 29.67 |
| 45 | ATOM | 2146 | CA  | THR | A | 276 | 17.225 | 45.198 | 54.996 | 1.00 | 30.47 |
|    | ATOM | 2147 | C   | THR | A | 276 | 17.120 | 46.624 | 55.597 | 1.00 | 34.60 |
|    | ATOM | 2148 | O   | THR | A | 276 | 17.766 | 47.588 | 55.129 | 1.00 | 31.01 |
|    | ATOM | 2149 | CB  | THR | A | 276 | 18.508 | 44.397 | 55.387 | 1.00 | 30.98 |
|    | ATOM | 2150 | OG1 | THR | A | 276 | 18.224 | 43.030 | 55.512 | 1.00 | 42.01 |
| 50 | ATOM | 2151 | CG2 | THR | A | 276 | 19.124 | 44.835 | 56.694 | 1.00 | 29.43 |
|    | ATOM | 2152 | N   | PHE | A | 277 | 16.280 | 46.759 | 56.622 | 1.00 | 27.69 |
|    | ATOM | 2153 | CA  | PHE | A | 277 | 16.164 | 48.034 | 57.274 | 1.00 | 28.92 |
|    | ATOM | 2154 | C   | PHE | A | 277 | 17.184 | 48.065 | 58.403 | 1.00 | 36.07 |
|    | ATOM | 2155 | O   | PHE | A | 277 | 17.337 | 47.088 | 59.131 | 1.00 | 34.57 |
| 55 | ATOM | 2156 | CB  | PHE | A | 277 | 14.791 | 48.265 | 57.901 | 1.00 | 30.17 |
|    | ATOM | 2157 | CG  | PHE | A | 277 | 13.774 | 48.458 | 56.848 | 1.00 | 30.72 |
|    | ATOM | 2158 | CD1 | PHE | A | 277 | 14.011 | 47.966 | 55.568 | 1.00 | 30.73 |
|    | ATOM | 2159 | CD2 | PHE | A | 277 | 12.573 | 49.114 | 57.105 | 1.00 | 30.61 |
|    | ATOM | 2160 | CE1 | PHE | A | 277 | 13.072 | 48.135 | 54.552 | 1.00 | 29.30 |
| 60 | ATOM | 2161 | CE2 | PHE | A | 277 | 11.619 | 49.276 | 56.101 | 1.00 | 32.26 |
|    | ATOM | 2162 | CZ  | PHE | A | 277 | 11.862 | 48.772 | 54.824 | 1.00 | 27.48 |
|    | ATOM | 2163 | N   | VAL | A | 278 | 17.864 | 49.186 | 58.562 | 1.00 | 32.97 |
|    | ATOM | 2164 | CA  | VAL | A | 278 | 18.839 | 49.338 | 59.614 | 1.00 | 32.66 |
|    | ATOM | 2165 | C   | VAL | A | 278 | 18.696 | 50.698 | 60.248 | 1.00 | 37.01 |
|    | ATOM | 2166 | O   | VAL | A | 278 | 18.251 | 51.635 | 59.599 | 1.00 | 37.16 |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
|    | ATOM | 2167 | CB  | VAL | A | 278 | 20.246 | 49.088 | 59.109 | 1.00 | 36.51 |
|    | ATOM | 2168 | CG1 | VAL | A | 278 | 20.173 | 47.967 | 58.086 | 1.00 | 37.40 |
|    | ATOM | 2169 | CG2 | VAL | A | 278 | 20.791 | 50.356 | 58.444 | 1.00 | 34.87 |
| 5  | ATOM | 2170 | N   | THR | A | 279 | 19.066 | 50.778 | 61.515 | 1.00 | 32.36 |
|    | ATOM | 2171 | CA  | THR | A | 279 | 18.948 | 51.994 | 62.264 | 1.00 | 31.03 |
|    | ATOM | 2172 | C   | THR | A | 279 | 20.121 | 52.883 | 62.035 | 1.00 | 37.42 |
|    | ATOM | 2173 | O   | THR | A | 279 | 21.243 | 52.397 | 61.920 | 1.00 | 39.87 |
|    | ATOM | 2174 | CB  | THR | A | 279 | 18.885 | 51.695 | 63.759 | 1.00 | 31.39 |
| 10 | ATOM | 2175 | OG1 | THR | A | 279 | 19.110 | 52.895 | 64.472 | 1.00 | 34.21 |
|    | ATOM | 2176 | CG2 | THR | A | 279 | 19.989 | 50.706 | 64.083 | 1.00 | 23.69 |
|    | ATOM | 2177 | N   | PRO | A | 280 | 19.845 | 54.187 | 62.000 | 1.00 | 30.07 |
|    | ATOM | 2178 | CA  | PRO | A | 280 | 20.903 | 55.132 | 61.802 | 1.00 | 27.00 |
|    | ATOM | 2179 | C   | PRO | A | 280 | 21.823 | 55.110 | 63.005 | 1.00 | 30.60 |
| 15 | ATOM | 2180 | O   | PRO | A | 280 | 22.951 | 55.588 | 62.934 | 1.00 | 30.20 |
|    | ATOM | 2181 | CB  | PRO | A | 280 | 20.249 | 56.497 | 61.601 | 1.00 | 26.23 |
|    | ATOM | 2182 | CG  | PRO | A | 280 | 18.769 | 56.337 | 61.889 | 1.00 | 28.07 |
|    | ATOM | 2183 | CD  | PRO | A | 280 | 18.499 | 54.848 | 61.984 | 1.00 | 26.11 |
|    | ATOM | 2184 | N   | THR | A | 281 | 21.348 | 54.509 | 64.112 | 1.00 | 27.82 |
| 20 | ATOM | 2185 | CA  | THR | A | 281 | 22.199 | 54.426 | 65.302 | 1.00 | 27.48 |
|    | ATOM | 2186 | C   | THR | A | 281 | 23.372 | 53.523 | 65.073 | 1.00 | 31.37 |
|    | ATOM | 2187 | O   | THR | A | 281 | 24.226 | 53.385 | 65.944 | 1.00 | 31.93 |
|    | ATOM | 2188 | CB  | THR | A | 281 | 21.499 | 54.016 | 66.601 | 1.00 | 21.45 |
|    | ATOM | 2189 | OG1 | THR | A | 281 | 21.021 | 52.681 | 66.524 | 1.00 | 33.18 |
| 25 | ATOM | 2190 | CG2 | THR | A | 281 | 20.388 | 54.994 | 66.874 | 1.00 | 9.89  |
|    | ATOM | 2191 | N   | LEU | A | 282 | 23.378 | 52.881 | 63.913 | 1.00 | 25.29 |
|    | ATOM | 2192 | CA  | LEU | A | 282 | 24.473 | 51.993 | 63.586 | 1.00 | 24.04 |
|    | ATOM | 2193 | C   | LEU | A | 282 | 25.682 | 52.790 | 63.049 | 1.00 | 34.74 |
|    | ATOM | 2194 | O   | LEU | A | 282 | 26.787 | 52.279 | 62.884 | 1.00 | 34.84 |
| 30 | ATOM | 2195 | CB  | LEU | A | 282 | 24.063 | 51.038 | 62.464 | 1.00 | 22.14 |
|    | ATOM | 2196 | CG  | LEU | A | 282 | 23.104 | 49.916 | 62.819 | 1.00 | 26.88 |
|    | ATOM | 2197 | CD1 | LEU | A | 282 | 23.312 | 48.809 | 61.791 | 1.00 | 27.77 |
|    | ATOM | 2198 | CD2 | LEU | A | 282 | 23.322 | 49.404 | 64.249 | 1.00 | 21.75 |
|    | ATOM | 2199 | N   | LEU | A | 283 | 25.465 | 54.063 | 62.744 | 1.00 | 32.05 |
| 35 | ATOM | 2200 | CA  | LEU | A | 283 | 26.501 | 54.903 | 62.159 | 1.00 | 31.43 |
|    | ATOM | 2201 | C   | LEU | A | 283 | 27.659 | 55.324 | 63.055 | 1.00 | 41.94 |
|    | ATOM | 2202 | O   | LEU | A | 283 | 27.907 | 56.525 | 63.196 | 1.00 | 49.19 |
|    | ATOM | 2203 | CB  | LEU | A | 283 | 25.861 | 56.117 | 61.418 | 1.00 | 29.55 |
|    | ATOM | 2204 | CG  | LEU | A | 283 | 24.720 | 55.661 | 60.488 | 1.00 | 32.94 |
| 40 | ATOM | 2205 | CD1 | LEU | A | 283 | 23.933 | 56.811 | 59.869 | 1.00 | 33.48 |
|    | ATOM | 2206 | CD2 | LEU | A | 283 | 25.232 | 54.716 | 59.409 | 1.00 | 28.39 |
|    | ATOM | 2207 | N   | ALA | A | 284 | 28.387 | 54.370 | 63.638 | 1.00 | 33.18 |
|    | ATOM | 2208 | CA  | ALA | A | 284 | 29.488 | 54.728 | 64.532 | 1.00 | 30.20 |
|    | ATOM | 2209 | C   | ALA | A | 284 | 30.655 | 55.492 | 63.922 | 1.00 | 31.97 |
| 45 | ATOM | 2210 | O   | ALA | A | 284 | 31.411 | 56.165 | 64.642 | 1.00 | 31.40 |
|    | ATOM | 2211 | CB  | ALA | A | 284 | 29.973 | 53.544 | 65.336 | 1.00 | 29.60 |
|    | ATOM | 2212 | N   | GLY | A | 285 | 30.801 | 55.371 | 62.605 | 1.00 | 27.10 |
|    | ATOM | 2213 | CA  | GLY | A | 285 | 31.882 | 56.018 | 61.867 | 1.00 | 29.77 |
|    | ATOM | 2214 | C   | GLY | A | 285 | 33.174 | 55.194 | 61.910 | 1.00 | 39.25 |
| 50 | ATOM | 2215 | O   | GLY | A | 285 | 34.264 | 55.649 | 61.544 | 1.00 | 41.21 |
|    | ATOM | 2216 | N   | ASP | A | 286 | 33.022 | 53.951 | 62.363 | 1.00 | 34.57 |
|    | ATOM | 2217 | CA  | ASP | A | 286 | 34.144 | 53.057 | 62.473 | 1.00 | 32.57 |
|    | ATOM | 2218 | C   | ASP | A | 286 | 33.805 | 51.625 | 62.130 | 1.00 | 31.59 |
|    | ATOM | 2219 | O   | ASP | A | 286 | 34.609 | 50.743 | 62.325 | 1.00 | 29.27 |
| 55 | ATOM | 2220 | CB  | ASP | A | 286 | 34.812 | 53.163 | 63.860 | 1.00 | 34.65 |
|    | ATOM | 2221 | CG  | ASP | A | 286 | 34.081 | 52.447 | 64.945 | 1.00 | 41.93 |
|    | ATOM | 2222 | OD1 | ASP | A | 286 | 33.008 | 51.893 | 64.765 | 1.00 | 45.21 |
|    | ATOM | 2223 | OD2 | ASP | A | 286 | 34.714 | 52.492 | 66.087 | 1.00 | 35.67 |
|    | ATOM | 2224 | N   | LYS | A | 287 | 32.590 | 51.395 | 61.641 | 1.00 | 29.46 |
| 60 | ATOM | 2225 | CA  | LYS | A | 287 | 32.199 | 50.038 | 61.272 | 1.00 | 31.62 |
|    | ATOM | 2226 | C   | LYS | A | 287 | 31.976 | 49.060 | 62.437 | 1.00 | 37.91 |
|    | ATOM | 2227 | O   | LYS | A | 287 | 31.761 | 47.879 | 62.240 | 1.00 | 37.91 |
|    | ATOM | 2228 | CB  | LYS | A | 287 | 33.215 | 49.447 | 60.304 | 1.00 | 32.17 |
|    | ATOM | 2229 | CG  | LYS | A | 287 | 33.510 | 50.358 | 59.119 | 1.00 | 51.60 |
|    | ATOM | 2230 | CD  | LYS | A | 287 | 33.960 | 49.601 | 57.877 | 1.00 | 50.74 |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
|    | ATOM | 2231 | CE  | LYS | A | 287 | 35.290 | 50.105 | 57.328 | 1.00 | 63.80 |
|    | ATOM | 2232 | NZ  | LYS | A | 287 | 35.167 | 50.866 | 56.069 | 1.00 | 71.91 |
|    | ATOM | 2233 | N   | SER | A | 288 | 32.168 | 49.575 | 63.647 | 1.00 | 31.58 |
| 5  | ATOM | 2234 | CA  | SER | A | 288 | 32.079 | 48.737 | 64.810 | 1.00 | 27.15 |
|    | ATOM | 2235 | C   | SER | A | 288 | 30.742 | 48.137 | 65.142 | 1.00 | 36.08 |
|    | ATOM | 2236 | O   | SER | A | 288 | 30.676 | 47.318 | 66.057 | 1.00 | 37.87 |
|    | ATOM | 2237 | CB  | SER | A | 288 | 32.618 | 49.463 | 66.005 | 1.00 | 16.31 |
|    | ATOM | 2238 | OG  | SER | A | 288 | 31.659 | 50.443 | 66.312 | 1.00 | 29.71 |
| 10 | ATOM | 2239 | N   | LEU | A | 289 | 29.669 | 48.529 | 64.460 | 1.00 | 29.34 |
|    | ATOM | 2240 | CA  | LEU | A | 289 | 28.351 | 47.979 | 64.794 | 1.00 | 24.70 |
|    | ATOM | 2241 | C   | LEU | A | 289 | 27.792 | 47.105 | 63.686 | 1.00 | 32.97 |
|    | ATOM | 2242 | O   | LEU | A | 289 | 26.591 | 46.766 | 63.648 | 1.00 | 30.35 |
|    | ATOM | 2243 | CB  | LEU | A | 289 | 27.385 | 49.090 | 65.191 | 1.00 | 21.45 |
|    | ATOM | 2244 | CG  | LEU | A | 289 | 27.954 | 49.887 | 66.347 | 1.00 | 22.99 |
| 15 | ATOM | 2245 | CD1 | LEU | A | 289 | 26.881 | 50.769 | 66.950 | 1.00 | 20.66 |
|    | ATOM | 2246 | CD2 | LEU | A | 289 | 28.381 | 48.881 | 67.394 | 1.00 | 29.65 |
|    | ATOM | 2247 | N   | SER | A | 290 | 28.723 | 46.753 | 62.801 | 1.00 | 31.21 |
|    | ATOM | 2248 | CA  | SER | A | 290 | 28.453 | 45.941 | 61.645 | 1.00 | 29.89 |
|    | ATOM | 2249 | C   | SER | A | 290 | 27.861 | 44.582 | 62.006 | 1.00 | 30.57 |
| 20 | ATOM | 2250 | O   | SER | A | 290 | 27.299 | 43.872 | 61.153 | 1.00 | 29.73 |
|    | ATOM | 2251 | CB  | SER | A | 290 | 29.704 | 45.800 | 60.783 | 1.00 | 29.27 |
|    | ATOM | 2252 | OG  | SER | A | 290 | 30.470 | 44.725 | 61.266 | 1.00 | 38.77 |
|    | ATOM | 2253 | N   | ASN | A | 291 | 27.980 | 44.207 | 63.282 | 1.00 | 26.55 |
| 25 | ATOM | 2254 | CA  | ASN | A | 291 | 27.449 | 42.909 | 63.706 | 1.00 | 25.78 |
|    | ATOM | 2255 | C   | ASN | A | 291 | 26.006 | 42.773 | 63.355 | 1.00 | 30.89 |
|    | ATOM | 2256 | O   | ASN | A | 291 | 25.576 | 41.702 | 62.975 | 1.00 | 29.73 |
|    | ATOM | 2257 | CB  | ASN | A | 291 | 27.725 | 42.503 | 65.157 | 1.00 | 28.48 |
|    | ATOM | 2258 | CG  | ASN | A | 291 | 26.910 | 43.313 | 66.119 | 1.00 | 33.33 |
|    | ATOM | 2259 | OD1 | ASN | A | 291 | 27.065 | 44.529 | 66.198 | 1.00 | 34.48 |
| 30 | ATOM | 2260 | ND2 | ASN | A | 291 | 26.001 | 42.653 | 66.818 | 1.00 | 28.96 |
|    | ATOM | 2261 | N   | VAL | A | 292 | 25.277 | 43.885 | 63.476 | 1.00 | 30.68 |
|    | ATOM | 2262 | CA  | VAL | A | 292 | 23.865 | 43.924 | 63.142 | 1.00 | 30.27 |
|    | ATOM | 2263 | C   | VAL | A | 292 | 23.667 | 43.619 | 61.669 | 1.00 | 32.61 |
| 35 | ATOM | 2264 | O   | VAL | A | 292 | 22.644 | 43.082 | 61.255 | 1.00 | 33.31 |
|    | ATOM | 2265 | CB  | VAL | A | 292 | 23.288 | 45.289 | 63.505 | 1.00 | 35.13 |
|    | ATOM | 2266 | CG1 | VAL | A | 292 | 21.877 | 45.486 | 62.946 | 1.00 | 33.48 |
|    | ATOM | 2267 | CG2 | VAL | A | 292 | 23.328 | 45.478 | 65.014 | 1.00 | 35.02 |
|    | ATOM | 2268 | N   | ILE | A | 293 | 24.653 | 43.975 | 60.861 | 1.00 | 27.92 |
| 40 | ATOM | 2269 | CA  | ILE | A | 293 | 24.527 | 43.685 | 59.461 | 1.00 | 28.71 |
|    | ATOM | 2270 | C   | ILE | A | 293 | 24.658 | 42.159 | 59.296 | 1.00 | 35.03 |
|    | ATOM | 2271 | O   | ILE | A | 293 | 23.860 | 41.475 | 58.624 | 1.00 | 38.34 |
|    | ATOM | 2272 | CB  | ILE | A | 293 | 25.554 | 44.438 | 58.606 | 1.00 | 33.84 |
|    | ATOM | 2273 | CG1 | ILE | A | 293 | 25.608 | 45.952 | 58.898 | 1.00 | 34.55 |
|    | ATOM | 2274 | CG2 | ILE | A | 293 | 25.305 | 44.186 | 57.121 | 1.00 | 36.50 |
| 45 | ATOM | 2275 | CD1 | ILE | A | 293 | 24.265 | 46.680 | 58.808 | 1.00 | 30.49 |
|    | ATOM | 2276 | N   | ALA | A | 294 | 25.668 | 41.584 | 59.934 | 1.00 | 23.76 |
|    | ATOM | 2277 | CA  | ALA | A | 294 | 25.836 | 40.138 | 59.809 | 1.00 | 19.95 |
|    | ATOM | 2278 | C   | ALA | A | 294 | 24.559 | 39.409 | 60.165 | 1.00 | 27.33 |
| 50 | ATOM | 2279 | O   | ALA | A | 294 | 24.183 | 38.422 | 59.505 | 1.00 | 25.48 |
|    | ATOM | 2280 | CB  | ALA | A | 294 | 26.984 | 39.644 | 60.688 | 1.00 | 19.24 |
|    | ATOM | 2281 | N   | HIS | A | 295 | 23.917 | 39.934 | 61.244 | 1.00 | 27.63 |
|    | ATOM | 2282 | CA  | HIS | A | 295 | 22.666 | 39.414 | 61.797 | 1.00 | 26.83 |
|    | ATOM | 2283 | C   | HIS | A | 295 | 21.611 | 39.383 | 60.734 | 1.00 | 28.61 |
| 55 | ATOM | 2284 | O   | HIS | A | 295 | 21.169 | 38.301 | 60.348 | 1.00 | 25.72 |
|    | ATOM | 2285 | CB  | HIS | A | 295 | 22.148 | 40.175 | 63.028 | 1.00 | 27.98 |
|    | ATOM | 2286 | CG  | HIS | A | 295 | 20.937 | 39.534 | 63.657 | 1.00 | 31.62 |
|    | ATOM | 2287 | ND1 | HIS | A | 295 | 21.047 | 38.675 | 64.763 | 1.00 | 32.66 |
|    | ATOM | 2288 | CD2 | HIS | A | 295 | 19.602 | 39.643 | 63.338 | 1.00 | 30.92 |
| 60 | ATOM | 2289 | CE1 | HIS | A | 295 | 19.802 | 38.298 | 65.088 | 1.00 | 30.14 |
|    | ATOM | 2290 | NE2 | HIS | A | 295 | 18.916 | 38.860 | 64.254 | 1.00 | 30.24 |
|    | ATOM | 2291 | N   | GLU | A | 296 | 21.257 | 40.590 | 60.251 | 1.00 | 27.23 |
|    | ATOM | 2292 | CA  | GLU | A | 296 | 20.266 | 40.749 | 59.195 | 1.00 | 25.98 |
|    | ATOM | 2293 | C   | GLU | A | 296 | 20.533 | 39.790 | 58.056 | 1.00 | 32.73 |
|    | ATOM | 2294 | O   | GLU | A | 296 | 19.628 | 39.081 | 57.561 | 1.00 | 31.88 |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
|    | ATOM | 2295 | CB  | GLU | A | 296 | 20.046 | 42.203 | 58.728 | 1.00 | 24.55 |
|    | ATOM | 2296 | CG  | GLU | A | 296 | 19.892 | 43.148 | 59.936 | 1.00 | 23.16 |
|    | ATOM | 2297 | CD  | GLU | A | 296 | 18.939 | 42.632 | 60.991 | 1.00 | 53.50 |
| 5  | ATOM | 2298 | OE1 | GLU | A | 296 | 17.964 | 41.956 | 60.700 | 1.00 | 23.99 |
|    | ATOM | 2299 | OE2 | GLU | A | 296 | 19.237 | 43.006 | 62.233 | 1.00 | 32.77 |
|    | ATOM | 2300 | N   | ILE | A | 297 | 21.803 | 39.745 | 57.675 | 1.00 | 25.37 |
|    | ATOM | 2301 | CA  | ILE | A | 297 | 22.195 | 38.870 | 56.599 | 1.00 | 22.64 |
|    | ATOM | 2302 | C   | ILE | A | 297 | 21.812 | 37.445 | 56.859 | 1.00 | 27.47 |
| 10 | ATOM | 2303 | O   | ILE | A | 297 | 21.175 | 36.799 | 56.048 | 1.00 | 26.25 |
|    | ATOM | 2304 | CB  | ILE | A | 297 | 23.672 | 38.963 | 56.302 | 1.00 | 24.19 |
|    | ATOM | 2305 | CG1 | ILE | A | 297 | 23.920 | 40.140 | 55.355 | 1.00 | 25.28 |
|    | ATOM | 2306 | CG2 | ILE | A | 297 | 24.079 | 37.686 | 55.626 | 1.00 | 20.77 |
|    | ATOM | 2307 | CD1 | ILE | A | 297 | 25.325 | 40.705 | 55.435 | 1.00 | 16.26 |
| 15 | ATOM | 2308 | N   | SER | A | 298 | 22.226 | 36.947 | 58.012 | 1.00 | 28.23 |
|    | ATOM | 2309 | CA  | SER | A | 298 | 21.939 | 35.569 | 58.377 | 1.00 | 25.04 |
|    | ATOM | 2310 | C   | SER | A | 298 | 20.467 | 35.235 | 58.298 | 1.00 | 26.21 |
|    | ATOM | 2311 | O   | SER | A | 298 | 20.118 | 34.097 | 58.000 | 1.00 | 26.30 |
|    | ATOM | 2312 | CB  | SER | A | 298 | 22.520 | 35.209 | 59.714 | 1.00 | 27.82 |
| 20 | ATOM | 2313 | OG  | SER | A | 298 | 23.890 | 35.552 | 59.714 | 1.00 | 35.98 |
|    | ATOM | 2314 | N   | HIS | A | 299 | 19.599 | 36.230 | 58.562 | 1.00 | 22.17 |
|    | ATOM | 2315 | CA  | HIS | A | 299 | 18.205 | 36.092 | 58.719 | 1.00 | 22.77 |
|    | ATOM | 2316 | C   | HIS | A | 299 | 17.614 | 35.710 | 57.387 | 1.00 | 29.10 |
|    | ATOM | 2317 | O   | HIS | A | 299 | 16.553 | 35.162 | 57.290 | 1.00 | 31.50 |
| 25 | ATOM | 2318 | CB  | HIS | A | 299 | 17.662 | 37.432 | 59.200 | 1.00 | 24.67 |
|    | ATOM | 2319 | CG  | HIS | A | 299 | 17.053 | 37.338 | 60.602 | 1.00 | 29.10 |
|    | ATOM | 2320 | ND1 | HIS | A | 299 | 16.190 | 36.368 | 60.975 | 1.00 | 30.70 |
|    | ATOM | 2321 | CD2 | HIS | A | 299 | 17.196 | 38.233 | 61.667 | 1.00 | 32.39 |
|    | ATOM | 2322 | CE1 | HIS | A | 299 | 15.811 | 36.675 | 62.233 | 1.00 | 30.41 |
| 30 | ATOM | 2323 | NE2 | HIS | A | 299 | 16.397 | 37.783 | 62.674 | 1.00 | 31.74 |
|    | ATOM | 2324 | N   | SER | A | 300 | 18.356 | 36.048 | 56.315 | 1.00 | 23.31 |
|    | ATOM | 2325 | CA  | SER | A | 300 | 17.942 | 35.581 | 55.010 | 1.00 | 24.24 |
|    | ATOM | 2326 | C   | SER | A | 300 | 17.879 | 34.050 | 54.977 | 1.00 | 34.13 |
|    | ATOM | 2327 | O   | SER | A | 300 | 17.075 | 33.463 | 54.305 | 1.00 | 33.28 |
| 35 | ATOM | 2328 | CB  | SER | A | 300 | 18.941 | 36.092 | 53.965 | 1.00 | 27.31 |
|    | ATOM | 2329 | OG  | SER | A | 300 | 18.947 | 37.519 | 53.962 | 1.00 | 49.96 |
|    | ATOM | 2330 | N   | TRP | A | 301 | 18.773 | 33.411 | 55.752 | 1.00 | 33.09 |
|    | ATOM | 2331 | CA  | TRP | A | 301 | 18.702 | 31.969 | 55.829 | 1.00 | 31.84 |
|    | ATOM | 2332 | C   | TRP | A | 301 | 17.740 | 31.511 | 56.895 | 1.00 | 32.15 |
| 40 | ATOM | 2333 | O   | TRP | A | 301 | 16.764 | 30.876 | 56.620 | 1.00 | 27.05 |
|    | ATOM | 2334 | CB  | TRP | A | 301 | 20.095 | 31.429 | 56.082 | 1.00 | 30.16 |
|    | ATOM | 2335 | CG  | TRP | A | 301 | 20.791 | 31.421 | 54.801 | 1.00 | 32.02 |
|    | ATOM | 2336 | CD1 | TRP | A | 301 | 20.787 | 30.393 | 53.859 | 1.00 | 35.05 |
|    | ATOM | 2337 | CD2 | TRP | A | 301 | 21.496 | 32.520 | 54.202 | 1.00 | 30.84 |
| 45 | ATOM | 2338 | NE1 | TRP | A | 301 | 21.415 | 30.732 | 52.722 | 1.00 | 33.29 |
|    | ATOM | 2339 | CE2 | TRP | A | 301 | 21.886 | 32.112 | 52.921 | 1.00 | 33.44 |
|    | ATOM | 2340 | CE3 | TRP | A | 301 | 21.811 | 33.790 | 54.631 | 1.00 | 32.65 |
|    | ATOM | 2341 | CZ2 | TRP | A | 301 | 22.577 | 32.970 | 52.108 | 1.00 | 32.21 |
|    | ATOM | 2342 | CZ3 | TRP | A | 301 | 22.503 | 34.652 | 53.812 | 1.00 | 36.10 |
| 50 | ATOM | 2343 | CH2 | TRP | A | 301 | 22.888 | 34.239 | 52.544 | 1.00 | 36.83 |
|    | ATOM | 2344 | N   | THR | A | 302 | 18.042 | 31.864 | 58.146 | 1.00 | 31.77 |
|    | ATOM | 2345 | CA  | THR | A | 302 | 17.125 | 31.488 | 59.215 | 1.00 | 33.55 |
|    | ATOM | 2346 | C   | THR | A | 302 | 16.276 | 32.690 | 59.695 | 1.00 | 36.35 |
|    | ATOM | 2347 | O   | THR | A | 302 | 16.759 | 33.590 | 60.330 | 1.00 | 36.56 |
| 55 | ATOM | 2348 | CB  | THR | A | 302 | 17.963 | 30.920 | 60.366 | 1.00 | 31.04 |
|    | ATOM | 2349 | OG1 | THR | A | 302 | 19.047 | 31.807 | 60.639 | 1.00 | 38.50 |
|    | ATOM | 2350 | CG2 | THR | A | 302 | 18.544 | 29.555 | 59.967 | 1.00 | 17.10 |
|    | ATOM | 2351 | N   | GLY | A | 303 | 15.053 | 32.418 | 59.250 | 1.00 | 25.28 |
|    | ATOM | 2352 | CA  | GLY | A | 303 | 13.908 | 33.236 | 59.483 | 1.00 | 21.59 |
|    | ATOM | 2353 | C   | GLY | A | 303 | 13.202 | 33.382 | 58.163 | 1.00 | 26.99 |
| 60 | ATOM | 2354 | O   | GLY | A | 303 | 12.040 | 33.040 | 57.994 | 1.00 | 26.18 |
|    | ATOM | 2355 | N   | ASN | A | 304 | 13.936 | 33.891 | 57.195 | 1.00 | 28.05 |
|    | ATOM | 2356 | CA  | ASN | A | 304 | 13.363 | 34.101 | 55.875 | 1.00 | 28.17 |
|    | ATOM | 2357 | C   | ASN | A | 304 | 13.141 | 32.839 | 55.056 | 1.00 | 28.99 |
|    | ATOM | 2358 | O   | ASN | A | 304 | 12.118 | 32.715 | 54.415 | 1.00 | 24.87 |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
|    | ATOM | 2359 | CB  | ASN | A | 304 | 14.091 | 35.176 | 55.047 | 1.00 | 23.55 |
|    | ATOM | 2360 | CG  | ASN | A | 304 | 14.133 | 36.499 | 55.757 | 1.00 | 37.80 |
|    | ATOM | 2361 | OD1 | ASN | A | 304 | 13.630 | 36.613 | 56.892 | 1.00 | 20.66 |
| 5  | ATOM | 2362 | ND2 | ASN | A | 304 | 14.752 | 37.488 | 55.093 | 1.00 | 24.17 |
|    | ATOM | 2363 | N   | LEU | A | 305 | 14.110 | 31.919 | 55.055 | 1.00 | 27.24 |
|    | ATOM | 2364 | CA  | LEU | A | 305 | 13.987 | 30.677 | 54.306 | 1.00 | 27.34 |
|    | ATOM | 2365 | C   | LEU | A | 305 | 13.218 | 29.665 | 55.121 | 1.00 | 31.29 |
|    | ATOM | 2366 | O   | LEU | A | 305 | 12.235 | 29.051 | 54.678 | 1.00 | 29.23 |
| 10 | ATOM | 2367 | CB  | LEU | A | 305 | 15.371 | 30.119 | 53.967 | 1.00 | 27.62 |
|    | ATOM | 2368 | CG  | LEU | A | 305 | 15.805 | 30.593 | 52.603 | 1.00 | 32.23 |
|    | ATOM | 2369 | CD1 | LEU | A | 305 | 17.289 | 30.293 | 52.412 | 1.00 | 28.91 |
|    | ATOM | 2370 | CD2 | LEU | A | 305 | 14.951 | 29.887 | 51.549 | 1.00 | 41.51 |
|    | ATOM | 2371 | N   | VAL | A | 306 | 13.711 | 29.528 | 56.347 | 1.00 | 27.75 |
| 15 | ATOM | 2372 | CA  | VAL | A | 306 | 13.134 | 28.652 | 57.327 | 1.00 | 29.99 |
|    | ATOM | 2373 | C   | VAL | A | 306 | 12.578 | 29.527 | 58.403 | 1.00 | 31.78 |
|    | ATOM | 2374 | O   | VAL | A | 306 | 13.306 | 30.217 | 59.110 | 1.00 | 28.32 |
|    | ATOM | 2375 | CB  | VAL | A | 306 | 14.092 | 27.593 | 57.827 | 1.00 | 37.24 |
|    | ATOM | 2376 | CG1 | VAL | A | 306 | 15.479 | 28.180 | 57.969 | 1.00 | 38.36 |
| 20 | ATOM | 2377 | CG2 | VAL | A | 306 | 13.602 | 27.107 | 59.164 | 1.00 | 37.56 |
|    | ATOM | 2378 | N   | THR | A | 307 | 11.259 | 29.517 | 58.440 | 1.00 | 29.40 |
|    | ATOM | 2379 | CA  | THR | A | 307 | 10.499 | 30.358 | 59.320 | 1.00 | 28.14 |
|    | ATOM | 2380 | C   | THR | A | 307 | 9.729  | 29.712 | 60.446 | 1.00 | 34.06 |
|    | ATOM | 2381 | O   | THR | A | 307 | 9.029  | 28.706 | 60.277 | 1.00 | 36.72 |
| 25 | ATOM | 2382 | CB  | THR | A | 307 | 9.474  | 31.115 | 58.460 | 1.00 | 23.03 |
|    | ATOM | 2383 | OG1 | THR | A | 307 | 10.124 | 31.811 | 57.422 | 1.00 | 28.56 |
|    | ATOM | 2384 | CG2 | THR | A | 307 | 8.665  | 32.068 | 59.336 | 1.00 | 12.55 |
|    | ATOM | 2385 | N   | ASN | A | 308 | 9.802  | 30.347 | 61.608 | 1.00 | 29.29 |
|    | ATOM | 2386 | CA  | ASN | A | 308 | 9.042  | 29.862 | 62.724 | 1.00 | 27.82 |
| 30 | ATOM | 2387 | C   | ASN | A | 308 | 7.576  | 29.716 | 62.234 | 1.00 | 31.42 |
|    | ATOM | 2388 | O   | ASN | A | 308 | 7.072  | 30.535 | 61.450 | 1.00 | 32.96 |
|    | ATOM | 2389 | CB  | ASN | A | 308 | 9.194  | 30.790 | 63.972 | 1.00 | 23.57 |
|    | ATOM | 2390 | CG  | ASN | A | 308 | 8.935  | 32.298 | 63.745 | 1.00 | 30.38 |
|    | ATOM | 2391 | OD1 | ASN | A | 308 | 9.505  | 33.190 | 64.400 | 1.00 | 23.70 |
| 35 | ATOM | 2392 | ND2 | ASN | A | 308 | 8.056  | 32.608 | 62.818 | 1.00 | 41.34 |
|    | ATOM | 2393 | N   | LYS | A | 309 | 6.890  | 28.658 | 62.640 | 1.00 | 24.10 |
|    | ATOM | 2394 | CA  | LYS | A | 309 | 5.502  | 28.433 | 62.230 | 1.00 | 23.40 |
|    | ATOM | 2395 | C   | LYS | A | 309 | 4.514  | 29.380 | 62.964 | 1.00 | 28.17 |
|    | ATOM | 2396 | O   | LYS | A | 309 | 3.430  | 29.756 | 62.474 | 1.00 | 22.88 |
| 40 | ATOM | 2397 | CB  | LYS | A | 309 | 5.151  | 26.975 | 62.459 | 1.00 | 24.26 |
|    | ATOM | 2398 | CG  | LYS | A | 309 | 4.036  | 26.478 | 61.555 | 1.00 | 28.57 |
|    | ATOM | 2399 | CD  | LYS | A | 309 | 3.543  | 25.075 | 61.924 | 1.00 | 38.25 |
|    | ATOM | 2400 | CE  | LYS | A | 309 | 3.475  | 24.112 | 60.739 | 1.00 | 78.39 |
|    | ATOM | 2401 | NZ  | LYS | A | 309 | 4.389  | 22.953 | 60.849 | 1.00 | 98.22 |
| 45 | ATOM | 2402 | N   | THR | A | 310 | 4.917  | 29.744 | 64.179 | 1.00 | 23.46 |
|    | ATOM | 2403 | CA  | THR | A | 310 | 4.179  | 30.616 | 65.037 | 1.00 | 22.98 |
|    | ATOM | 2404 | C   | THR | A | 310 | 5.142  | 31.336 | 65.922 | 1.00 | 31.43 |
|    | ATOM | 2405 | O   | THR | A | 310 | 6.223  | 30.836 | 66.230 | 1.00 | 31.51 |
|    | ATOM | 2406 | CB  | THR | A | 310 | 3.104  | 29.917 | 65.871 | 1.00 | 34.01 |
| 50 | ATOM | 2407 | OG1 | THR | A | 310 | 3.684  | 29.148 | 66.945 | 1.00 | 27.97 |
|    | ATOM | 2408 | CG2 | THR | A | 310 | 2.174  | 29.114 | 64.956 | 1.00 | 24.58 |
|    | ATOM | 2409 | N   | TRP | A | 311 | 4.733  | 32.527 | 66.299 | 1.00 | 29.82 |
|    | ATOM | 2410 | CA  | TRP | A | 311 | 5.559  | 33.371 | 67.120 | 1.00 | 30.49 |
|    | ATOM | 2411 | C   | TRP | A | 311 | 6.044  | 32.692 | 68.381 | 1.00 | 26.99 |
| 55 | ATOM | 2412 | O   | TRP | A | 311 | 7.015  | 33.101 | 68.971 | 1.00 | 25.15 |
|    | ATOM | 2413 | CB  | TRP | A | 311 | 4.933  | 34.768 | 67.320 | 1.00 | 30.34 |
|    | ATOM | 2414 | CG  | TRP | A | 311 | 4.706  | 35.412 | 66.001 | 1.00 | 30.63 |
|    | ATOM | 2415 | CD1 | TRP | A | 311 | 3.514  | 35.785 | 65.490 | 1.00 | 32.07 |
|    | ATOM | 2416 | CD2 | TRP | A | 311 | 5.705  | 35.723 | 65.008 | 1.00 | 31.31 |
| 60 | ATOM | 2417 | NE1 | TRP | A | 311 | 3.703  | 36.335 | 64.250 | 1.00 | 29.97 |
|    | ATOM | 2418 | CE2 | TRP | A | 311 | 5.033  | 36.317 | 63.931 | 1.00 | 32.88 |
|    | ATOM | 2419 | CE3 | TRP | A | 311 | 7.099  | 35.586 | 64.943 | 1.00 | 31.44 |
|    | ATOM | 2420 | CZ2 | TRP | A | 311 | 5.721  | 36.771 | 62.804 | 1.00 | 31.56 |
|    | ATOM | 2421 | CZ3 | TRP | A | 311 | 7.779  | 36.059 | 63.848 | 1.00 | 30.39 |
|    | ATOM | 2422 | CH2 | TRP | A | 311 | 7.089  | 36.639 | 62.789 | 1.00 | 30.58 |



|    |      |      |     |           |        |        |        |      |       |
|----|------|------|-----|-----------|--------|--------|--------|------|-------|
|    | ATOM | 2423 | N   | ASP A 312 | 5.366  | 31.632 | 68.770 | 1.00 | 27.36 |
|    | ATOM | 2424 | CA  | ASP A 312 | 5.757  | 30.868 | 69.950 | 1.00 | 27.38 |
|    | ATOM | 2425 | C   | ASP A 312 | 7.149  | 30.213 | 69.757 | 1.00 | 31.25 |
|    | ATOM | 2426 | O   | ASP A 312 | 7.826  | 29.802 | 70.718 | 1.00 | 27.07 |
| 5  | ATOM | 2427 | CB  | ASP A 312 | 4.697  | 29.750 | 70.217 | 1.00 | 25.96 |
|    | ATOM | 2428 | CG  | ASP A 312 | 3.432  | 30.230 | 70.872 | 1.00 | 27.42 |
|    | ATOM | 2429 | OD1 | ASP A 312 | 3.197  | 31.396 | 71.102 | 1.00 | 28.97 |
|    | ATOM | 2430 | OD2 | ASP A 312 | 2.623  | 29.265 | 71.208 | 1.00 | 29.33 |
| 10 | ATOM | 2431 | N   | HIS A 313 | 7.562  | 30.089 | 68.487 | 1.00 | 25.04 |
|    | ATOM | 2432 | CA  | HIS A 313 | 8.820  | 29.454 | 68.164 | 1.00 | 23.48 |
|    | ATOM | 2433 | C   | HIS A 313 | 9.864  | 30.452 | 67.737 | 1.00 | 25.38 |
|    | ATOM | 2434 | O   | HIS A 313 | 10.929 | 30.139 | 67.214 | 1.00 | 29.97 |
|    | ATOM | 2435 | CB  | HIS A 313 | 8.588  | 28.245 | 67.209 | 1.00 | 25.00 |
|    | ATOM | 2436 | CG  | HIS A 313 | 7.641  | 27.230 | 67.837 | 1.00 | 29.77 |
| 15 | ATOM | 2437 | ND1 | HIS A 313 | 8.087  | 26.183 | 68.635 | 1.00 | 31.37 |
|    | ATOM | 2438 | CD2 | HIS A 313 | 6.279  | 27.152 | 67.808 | 1.00 | 31.31 |
|    | ATOM | 2439 | CE1 | HIS A 313 | 7.015  | 25.509 | 69.039 | 1.00 | 28.91 |
|    | ATOM | 2440 | NE2 | HIS A 313 | 5.913  | 26.066 | 68.559 | 1.00 | 29.40 |
|    | ATOM | 2441 | N   | PHE A 314 | 9.521  | 31.682 | 68.005 | 1.00 | 17.43 |
| 20 | ATOM | 2442 | CA  | PHE A 314 | 10.345 | 32.810 | 67.701 | 1.00 | 17.16 |
|    | ATOM | 2443 | C   | PHE A 314 | 11.852 | 32.523 | 67.812 | 1.00 | 26.01 |
|    | ATOM | 2444 | O   | PHE A 314 | 12.669 | 32.922 | 66.963 | 1.00 | 30.40 |
|    | ATOM | 2445 | CB  | PHE A 314 | 9.908  | 34.056 | 68.517 | 1.00 | 18.63 |
|    | ATOM | 2446 | CG  | PHE A 314 | 10.592 | 35.351 | 68.113 | 1.00 | 20.10 |
| 25 | ATOM | 2447 | CD1 | PHE A 314 | 10.712 | 35.697 | 66.768 | 1.00 | 21.80 |
|    | ATOM | 2448 | CD2 | PHE A 314 | 11.129 | 36.214 | 69.070 | 1.00 | 22.60 |
|    | ATOM | 2449 | CE1 | PHE A 314 | 11.337 | 36.890 | 66.400 | 1.00 | 24.74 |
|    | ATOM | 2450 | CE2 | PHE A 314 | 11.750 | 37.416 | 68.716 | 1.00 | 27.24 |
|    | ATOM | 2451 | CZ  | PHE A 314 | 11.857 | 37.756 | 67.368 | 1.00 | 24.97 |
| 30 | ATOM | 2452 | N   | TRP A 315 | 12.235 | 31.828 | 68.861 | 1.00 | 19.66 |
|    | ATOM | 2453 | CA  | TRP A 315 | 13.639 | 31.541 | 69.068 | 1.00 | 17.87 |
|    | ATOM | 2454 | C   | TRP A 315 | 14.292 | 30.775 | 67.953 | 1.00 | 28.55 |
|    | ATOM | 2455 | O   | TRP A 315 | 15.518 | 30.769 | 67.830 | 1.00 | 29.23 |
|    | ATOM | 2456 | CB  | TRP A 315 | 13.860 | 30.842 | 70.362 | 1.00 | 16.03 |
| 35 | ATOM | 2457 | CG  | TRP A 315 | 13.613 | 29.408 | 70.161 | 1.00 | 19.64 |
|    | ATOM | 2458 | CD1 | TRP A 315 | 12.428 | 28.787 | 70.247 | 1.00 | 22.39 |
|    | ATOM | 2459 | CD2 | TRP A 315 | 14.599 | 28.430 | 69.876 | 1.00 | 21.70 |
|    | ATOM | 2460 | NE1 | TRP A 315 | 12.597 | 27.457 | 70.033 | 1.00 | 24.22 |
|    | ATOM | 2461 | CE2 | TRP A 315 | 13.934 | 27.205 | 69.801 | 1.00 | 27.96 |
| 40 | ATOM | 2462 | CE3 | TRP A 315 | 15.976 | 28.481 | 69.681 | 1.00 | 22.89 |
|    | ATOM | 2463 | CZ2 | TRP A 315 | 14.631 | 26.018 | 69.547 | 1.00 | 27.76 |
|    | ATOM | 2464 | CZ3 | TRP A 315 | 16.651 | 27.321 | 69.421 | 1.00 | 23.16 |
|    | ATOM | 2465 | CH2 | TRP A 315 | 15.991 | 26.108 | 69.341 | 1.00 | 23.94 |
|    | ATOM | 2466 | N   | LEU A 316 | 13.488 | 30.114 | 67.144 | 1.00 | 26.33 |
| 45 | ATOM | 2467 | CA  | LEU A 316 | 14.092 | 29.400 | 66.067 | 1.00 | 25.44 |
|    | ATOM | 2468 | C   | LEU A 316 | 14.666 | 30.443 | 65.129 | 1.00 | 33.21 |
|    | ATOM | 2469 | O   | LEU A 316 | 15.737 | 30.252 | 64.530 | 1.00 | 37.80 |
|    | ATOM | 2470 | CB  | LEU A 316 | 13.050 | 28.567 | 65.311 | 1.00 | 24.82 |
|    | ATOM | 2471 | CG  | LEU A 316 | 12.663 | 27.242 | 65.956 | 1.00 | 27.62 |
| 50 | ATOM | 2472 | CD1 | LEU A 316 | 11.574 | 26.552 | 65.106 | 1.00 | 22.30 |
|    | ATOM | 2473 | CD2 | LEU A 316 | 13.897 | 26.344 | 66.097 | 1.00 | 27.03 |
|    | ATOM | 2474 | N   | ASN A 317 | 13.931 | 31.555 | 64.997 | 1.00 | 20.55 |
|    | ATOM | 2475 | CA  | ASN A 317 | 14.354 | 32.624 | 64.115 | 1.00 | 19.34 |
|    | ATOM | 2476 | C   | ASN A 317 | 15.603 | 33.333 | 64.531 | 1.00 | 30.38 |
| 55 | ATOM | 2477 | O   | ASN A 317 | 16.553 | 33.425 | 63.766 | 1.00 | 32.04 |
|    | ATOM | 2478 | CB  | ASN A 317 | 13.273 | 33.682 | 63.838 | 1.00 | 14.82 |
|    | ATOM | 2479 | CG  | ASN A 317 | 12.330 | 33.177 | 62.793 | 1.00 | 31.14 |
|    | ATOM | 2480 | OD1 | ASN A 317 | 12.151 | 31.966 | 62.657 | 1.00 | 38.42 |
|    | ATOM | 2481 | ND2 | ASN A 317 | 11.724 | 34.074 | 62.049 | 1.00 | 17.34 |
| 60 | ATOM | 2482 | N   | GLU A 318 | 15.562 | 33.870 | 65.750 | 1.00 | 26.15 |
|    | ATOM | 2483 | CA  | GLU A 318 | 16.624 | 34.648 | 66.358 | 1.00 | 20.23 |
|    | ATOM | 2484 | C   | GLU A 318 | 17.860 | 33.884 | 66.816 | 1.00 | 23.53 |
|    | ATOM | 2485 | O   | GLU A 318 | 19.006 | 34.273 | 66.554 | 1.00 | 26.34 |
|    | ATOM | 2486 | CB  | GLU A 318 | 15.998 | 35.484 | 67.456 | 1.00 | 19.11 |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
|    | ATOM | 2487 | CG  | GLU | A | 318 | 14.999 | 36.480 | 66.800 | 1.00 | 24.06 |
|    | ATOM | 2488 | CD  | GLU | A | 318 | 15.615 | 37.391 | 65.758 | 1.00 | 40.32 |
|    | ATOM | 2489 | OE1 | GLU | A | 318 | 16.833 | 37.559 | 65.612 | 1.00 | 21.24 |
| 5  | ATOM | 2490 | OE2 | GLU | A | 318 | 14.703 | 38.025 | 65.062 | 1.00 | 24.23 |
|    | ATOM | 2491 | N   | GLY | A | 319 | 17.621 | 32.782 | 67.494 | 1.00 | 17.17 |
|    | ATOM | 2492 | CA  | GLY | A | 319 | 18.681 | 31.955 | 68.016 | 1.00 | 15.31 |
|    | ATOM | 2493 | C   | GLY | A | 319 | 19.673 | 31.601 | 66.953 | 1.00 | 24.07 |
|    | ATOM | 2494 | O   | GLY | A | 319 | 20.860 | 31.897 | 67.080 | 1.00 | 28.47 |
| 10 | ATOM | 2495 | N   | HIS | A | 320 | 19.165 | 30.956 | 65.907 | 1.00 | 20.24 |
|    | ATOM | 2496 | CA  | HIS | A | 320 | 19.977 | 30.556 | 64.790 | 1.00 | 20.13 |
|    | ATOM | 2497 | C   | HIS | A | 320 | 20.678 | 31.759 | 64.142 | 1.00 | 24.97 |
|    | ATOM | 2498 | O   | HIS | A | 320 | 21.855 | 31.700 | 63.739 | 1.00 | 23.54 |
|    | ATOM | 2499 | CB  | HIS | A | 320 | 19.143 | 29.737 | 63.791 | 1.00 | 20.57 |
| 15 | ATOM | 2500 | CG  | HIS | A | 320 | 18.662 | 28.426 | 64.349 | 1.00 | 22.57 |
|    | ATOM | 2501 | ND1 | HIS | A | 320 | 17.471 | 28.332 | 65.058 | 1.00 | 22.98 |
|    | ATOM | 2502 | CD2 | HIS | A | 320 | 19.217 | 27.176 | 64.286 | 1.00 | 19.52 |
|    | ATOM | 2503 | CE1 | HIS | A | 320 | 17.336 | 27.046 | 65.385 | 1.00 | 19.18 |
|    | ATOM | 2504 | NE2 | HIS | A | 320 | 18.368 | 26.329 | 64.952 | 1.00 | 18.12 |
| 20 | ATOM | 2505 | N   | THR | A | 321 | 19.958 | 32.875 | 64.053 | 1.00 | 21.61 |
|    | ATOM | 2506 | CA  | THR | A | 321 | 20.543 | 34.056 | 63.478 | 1.00 | 22.16 |
|    | ATOM | 2507 | C   | THR | A | 321 | 21.697 | 34.552 | 64.342 | 1.00 | 27.47 |
|    | ATOM | 2508 | O   | THR | A | 321 | 22.789 | 34.825 | 63.836 | 1.00 | 26.64 |
|    | ATOM | 2509 | CB  | THR | A | 321 | 19.470 | 35.097 | 63.113 | 1.00 | 27.88 |
| 25 | ATOM | 2510 | OG1 | THR | A | 321 | 18.403 | 34.392 | 62.523 | 1.00 | 27.92 |
|    | ATOM | 2511 | CG2 | THR | A | 321 | 19.999 | 36.088 | 62.087 | 1.00 | 18.05 |
|    | ATOM | 2512 | N   | VAL | A | 322 | 21.496 | 34.634 | 65.659 | 1.00 | 21.90 |
|    | ATOM | 2513 | CA  | VAL | A | 322 | 22.610 | 35.054 | 66.470 | 1.00 | 19.44 |
|    | ATOM | 2514 | C   | VAL | A | 322 | 23.762 | 34.071 | 66.285 | 1.00 | 24.43 |
| 30 | ATOM | 2515 | O   | VAL | A | 322 | 24.926 | 34.414 | 66.188 | 1.00 | 21.48 |
|    | ATOM | 2516 | CB  | VAL | A | 322 | 22.218 | 35.185 | 67.928 | 1.00 | 20.92 |
|    | ATOM | 2517 | CG1 | VAL | A | 322 | 23.406 | 35.644 | 68.772 | 1.00 | 18.37 |
|    | ATOM | 2518 | CG2 | VAL | A | 322 | 21.093 | 36.200 | 68.048 | 1.00 | 20.01 |
|    | ATOM | 2519 | N   | TYR | A | 323 | 23.427 | 32.811 | 66.197 | 1.00 | 27.08 |
| 35 | ATOM | 2520 | CA  | TYR | A | 323 | 24.446 | 31.803 | 66.013 | 1.00 | 26.26 |
|    | ATOM | 2521 | C   | TYR | A | 323 | 25.222 | 32.036 | 64.728 | 1.00 | 28.26 |
|    | ATOM | 2522 | O   | TYR | A | 323 | 26.431 | 31.894 | 64.643 | 1.00 | 27.51 |
|    | ATOM | 2523 | CB  | TYR | A | 323 | 23.804 | 30.407 | 66.020 | 1.00 | 25.74 |
|    | ATOM | 2524 | CG  | TYR | A | 323 | 24.867 | 29.341 | 65.987 | 1.00 | 26.66 |
| 40 | ATOM | 2525 | CD1 | TYR | A | 323 | 25.539 | 28.957 | 67.150 | 1.00 | 29.09 |
|    | ATOM | 2526 | CD2 | TYR | A | 323 | 25.199 | 28.713 | 64.789 | 1.00 | 24.52 |
|    | ATOM | 2527 | CE1 | TYR | A | 323 | 26.530 | 27.974 | 67.157 | 1.00 | 22.56 |
|    | ATOM | 2528 | CE2 | TYR | A | 323 | 26.178 | 27.722 | 64.770 | 1.00 | 25.31 |
|    | ATOM | 2529 | CZ  | TYR | A | 323 | 26.846 | 27.370 | 65.944 | 1.00 | 29.19 |
| 45 | ATOM | 2530 | OH  | TYR | A | 323 | 27.823 | 26.434 | 65.895 | 1.00 | 27.51 |
|    | ATOM | 2531 | N   | LEU | A | 324 | 24.497 | 32.408 | 63.702 | 1.00 | 24.82 |
|    | ATOM | 2532 | CA  | LEU | A | 324 | 25.135 | 32.638 | 62.439 | 1.00 | 26.04 |
|    | ATOM | 2533 | C   | LEU | A | 324 | 25.832 | 33.952 | 62.417 | 1.00 | 30.92 |
|    | ATOM | 2534 | O   | LEU | A | 324 | 26.903 | 34.045 | 61.851 | 1.00 | 33.76 |
| 50 | ATOM | 2535 | CB  | LEU | A | 324 | 24.176 | 32.537 | 61.235 | 1.00 | 26.21 |
|    | ATOM | 2536 | CG  | LEU | A | 324 | 23.916 | 31.112 | 60.778 | 1.00 | 28.46 |
|    | ATOM | 2537 | CD1 | LEU | A | 324 | 22.752 | 31.109 | 59.791 | 1.00 | 28.95 |
|    | ATOM | 2538 | CD2 | LEU | A | 324 | 25.169 | 30.508 | 60.151 | 1.00 | 26.54 |
|    | ATOM | 2539 | N   | GLU | A | 325 | 25.234 | 34.976 | 63.033 | 1.00 | 27.04 |
| 55 | ATOM | 2540 | CA  | GLU | A | 325 | 25.870 | 36.303 | 63.064 | 1.00 | 22.88 |
|    | ATOM | 2541 | C   | GLU | A | 325 | 27.282 | 36.210 | 63.624 | 1.00 | 28.76 |
|    | ATOM | 2542 | O   | GLU | A | 325 | 28.250 | 36.722 | 63.026 | 1.00 | 26.24 |
|    | ATOM | 2543 | CB  | GLU | A | 325 | 25.016 | 37.365 | 63.759 | 1.00 | 22.01 |
|    | ATOM | 2544 | CG  | GLU | A | 325 | 25.827 | 38.411 | 64.524 | 1.00 | 41.55 |
| 60 | ATOM | 2545 | CD  | GLU | A | 325 | 25.035 | 39.040 | 65.646 | 1.00 | 72.11 |
|    | ATOM | 2546 | OE1 | GLU | A | 325 | 23.866 | 38.764 | 65.862 | 1.00 | 41.88 |
|    | ATOM | 2547 | OE2 | GLU | A | 325 | 25.719 | 39.922 | 66.350 | 1.00 | 67.15 |
|    | ATOM | 2548 | N   | ARG | A | 326 | 27.349 | 35.479 | 64.755 | 1.00 | 27.84 |
|    | ATOM | 2549 | CA  | ARG | A | 326 | 28.551 | 35.213 | 65.511 | 1.00 | 28.10 |
|    | ATOM | 2550 | C   | ARG | A | 326 | 29.604 | 34.457 | 64.771 | 1.00 | 30.90 |



|    |      |      |     |     |   |     |        |        |        |      |        |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
|    | ATOM | 2551 | O   | ARG | A | 326 | 30.763 | 34.747 | 64.976 | 1.00 | 33.93  |
|    | ATOM | 2552 | CB  | ARG | A | 326 | 28.334 | 34.761 | 66.947 | 1.00 | 31.52  |
|    | ATOM | 2553 | CG  | ARG | A | 326 | 27.645 | 35.864 | 67.726 | 1.00 | 22.20  |
| 5  | ATOM | 2554 | CD  | ARG | A | 326 | 27.462 | 35.572 | 69.203 | 1.00 | 28.71  |
|    | ATOM | 2555 | NE  | ARG | A | 326 | 26.727 | 36.673 | 69.830 | 1.00 | 23.82  |
|    | ATOM | 2556 | CZ  | ARG | A | 326 | 25.805 | 36.556 | 70.780 | 1.00 | 26.09  |
|    | ATOM | 2557 | NH1 | ARG | A | 326 | 25.443 | 35.388 | 71.305 | 1.00 | 23.16  |
|    | ATOM | 2558 | NH2 | ARG | A | 326 | 25.220 | 37.655 | 71.222 | 1.00 | 24.77  |
| 10 | ATOM | 2559 | N   | HIS | A | 327 | 29.221 | 33.511 | 63.918 | 1.00 | 29.85  |
|    | ATOM | 2560 | CA  | HIS | A | 327 | 30.207 | 32.777 | 63.120 | 1.00 | 30.52  |
|    | ATOM | 2561 | C   | HIS | A | 327 | 30.778 | 33.738 | 62.085 | 1.00 | 35.50  |
|    | ATOM | 2562 | O   | HIS | A | 327 | 31.966 | 33.777 | 61.822 | 1.00 | 36.74  |
|    | ATOM | 2563 | CB  | HIS | A | 327 | 29.591 | 31.555 | 62.407 | 1.00 | 31.59  |
|    | ATOM | 2564 | CG  | HIS | A | 327 | 29.764 | 30.259 | 63.176 | 1.00 | 34.51  |
| 15 | ATOM | 2565 | ND1 | HIS | A | 327 | 30.963 | 29.913 | 63.788 | 1.00 | 36.17  |
|    | ATOM | 2566 | CD2 | HIS | A | 327 | 28.875 | 29.263 | 63.432 | 1.00 | 35.58  |
|    | ATOM | 2567 | CE1 | HIS | A | 327 | 30.778 | 28.740 | 64.384 | 1.00 | 35.27  |
|    | ATOM | 2568 | NE2 | HIS | A | 327 | 29.532 | 28.322 | 64.191 | 1.00 | 35.56  |
| 20 | ATOM | 2569 | N   | ILE | A | 328 | 29.902 | 34.549 | 61.511 | 1.00 | 31.10  |
|    | ATOM | 2570 | CA  | ILE | A | 328 | 30.328 | 35.517 | 60.528 | 1.00 | 31.66  |
|    | ATOM | 2571 | C   | ILE | A | 328 | 31.416 | 36.407 | 61.086 | 1.00 | 40.12  |
|    | ATOM | 2572 | O   | ILE | A | 328 | 32.451 | 36.615 | 60.465 | 1.00 | 40.81  |
|    | ATOM | 2573 | CB  | ILE | A | 328 | 29.175 | 36.379 | 59.998 | 1.00 | 32.94  |
|    | ATOM | 2574 | CG1 | ILE | A | 328 | 28.220 | 35.570 | 59.114 | 1.00 | 29.53  |
| 25 | ATOM | 2575 | CG2 | ILE | A | 328 | 29.694 | 37.591 | 59.201 | 1.00 | 30.91  |
|    | ATOM | 2576 | CD1 | ILE | A | 328 | 27.119 | 36.463 | 58.535 | 1.00 | 32.98  |
|    | ATOM | 2577 | N   | CYS | A | 329 | 31.179 | 36.948 | 62.266 | 1.00 | 37.88  |
|    | ATOM | 2578 | CA  | CYS | A | 329 | 32.170 | 37.810 | 62.851 | 1.00 | 39.54  |
|    | ATOM | 2579 | C   | CYS | A | 329 | 33.475 | 37.092 | 63.157 | 1.00 | 40.19  |
| 30 | ATOM | 2580 | O   | CYS | A | 329 | 34.567 | 37.642 | 62.971 | 1.00 | 38.44  |
|    | ATOM | 2581 | CB  | CYS | A | 329 | 31.607 | 38.509 | 64.083 | 1.00 | 42.61  |
|    | ATOM | 2582 | SG  | CYS | A | 329 | 30.241 | 39.595 | 63.619 | 1.00 | 48.14  |
|    | ATOM | 2583 | N   | GLY | A | 330 | 33.332 | 35.852 | 63.632 | 1.00 | 34.74  |
| 35 | ATOM | 2584 | CA  | GLY | A | 330 | 34.471 | 35.030 | 63.980 | 1.00 | 35.20  |
|    | ATOM | 2585 | C   | GLY | A | 330 | 35.359 | 34.854 | 62.778 | 1.00 | 43.66  |
|    | ATOM | 2586 | O   | GLY | A | 330 | 36.581 | 34.857 | 62.891 | 1.00 | 46.79  |
|    | ATOM | 2587 | N   | ARG | A | 331 | 34.709 | 34.725 | 61.622 | 1.00 | 34.99  |
|    | ATOM | 2588 | CA  | ARG | A | 331 | 35.416 | 34.562 | 60.392 | 1.00 | 33.19  |
|    | ATOM | 2589 | C   | ARG | A | 331 | 36.086 | 35.863 | 60.017 | 1.00 | 40.63  |
| 40 | ATOM | 2590 | O   | ARG | A | 331 | 37.238 | 35.914 | 59.586 | 1.00 | 44.40  |
|    | ATOM | 2591 | CB  | ARG | A | 331 | 34.494 | 34.101 | 59.269 | 1.00 | 31.29  |
|    | ATOM | 2592 | CG  | ARG | A | 331 | 33.987 | 32.685 | 59.450 | 1.00 | 47.66  |
|    | ATOM | 2593 | CD  | ARG | A | 331 | 34.812 | 31.722 | 58.622 | 1.00 | 70.36  |
|    | ATOM | 2594 | NE  | ARG | A | 331 | 34.461 | 31.851 | 57.221 | 1.00 | 80.25  |
| 45 | ATOM | 2595 | CZ  | ARG | A | 331 | 33.615 | 31.023 | 56.628 | 1.00 | 100.00 |
|    | ATOM | 2596 | NH1 | ARG | A | 331 | 33.055 | 29.999 | 57.279 | 1.00 | 79.12  |
|    | ATOM | 2597 | NH2 | ARG | A | 331 | 33.334 | 31.216 | 55.341 | 1.00 | 89.33  |
|    | ATOM | 2598 | N   | LEU | A | 332 | 35.342 | 36.926 | 60.172 | 1.00 | 32.14  |
| 50 | ATOM | 2599 | CA  | LEU | A | 332 | 35.885 | 38.198 | 59.820 | 1.00 | 30.02  |
|    | ATOM | 2600 | C   | LEU | A | 332 | 37.013 | 38.612 | 60.761 | 1.00 | 40.33  |
|    | ATOM | 2601 | O   | LEU | A | 332 | 38.084 | 38.972 | 60.286 | 1.00 | 40.10  |
|    | ATOM | 2602 | CB  | LEU | A | 332 | 34.772 | 39.262 | 59.822 | 1.00 | 28.20  |
|    | ATOM | 2603 | CG  | LEU | A | 332 | 34.451 | 39.896 | 58.469 | 1.00 | 28.82  |
|    | ATOM | 2604 | CD1 | LEU | A | 332 | 35.007 | 39.063 | 57.341 | 1.00 | 23.73  |
| 55 | ATOM | 2605 | CD2 | LEU | A | 332 | 32.947 | 40.114 | 58.306 | 1.00 | 29.76  |
|    | ATOM | 2606 | N   | PHE | A | 333 | 36.744 | 38.557 | 62.091 | 1.00 | 37.69  |
|    | ATOM | 2607 | CA  | PHE | A | 333 | 37.657 | 38.997 | 63.143 | 1.00 | 34.12  |
|    | ATOM | 2608 | C   | PHE | A | 333 | 38.251 | 37.956 | 64.035 | 1.00 | 37.99  |
|    | ATOM | 2609 | O   | PHE | A | 333 | 39.015 | 38.293 | 64.925 | 1.00 | 41.67  |
| 60 | ATOM | 2610 | CB  | PHE | A | 333 | 36.970 | 40.058 | 64.024 | 1.00 | 35.62  |
|    | ATOM | 2611 | CG  | PHE | A | 333 | 36.209 | 41.003 | 63.138 | 1.00 | 39.09  |
|    | ATOM | 2612 | CD1 | PHE | A | 333 | 36.887 | 41.923 | 62.332 | 1.00 | 43.22  |
|    | ATOM | 2613 | CD2 | PHE | A | 333 | 34.818 | 40.941 | 63.045 | 1.00 | 42.78  |
|    | ATOM | 2614 | CE1 | PHE | A | 333 | 36.205 | 42.781 | 61.464 | 1.00 | 44.14  |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
|    | ATOM | 2615 | CE2 | PHE | A | 333 | 34.123 | 41.806 | 62.194 | 1.00 | 46.56 |
|    | ATOM | 2616 | CZ  | PHE | A | 333 | 34.814 | 42.716 | 61.389 | 1.00 | 43.20 |
|    | ATOM | 2617 | N   | GLY | A | 334 | 37.908 | 36.706 | 63.865 | 1.00 | 34.36 |
| 5  | ATOM | 2618 | CA  | GLY | A | 334 | 38.507 | 35.705 | 64.763 | 1.00 | 32.89 |
|    | ATOM | 2619 | C   | GLY | A | 334 | 37.582 | 34.985 | 65.767 | 1.00 | 32.67 |
|    | ATOM | 2620 | O   | GLY | A | 334 | 36.641 | 35.540 | 66.340 | 1.00 | 33.48 |
|    | ATOM | 2621 | N   | GLU | A | 335 | 37.908 | 33.726 | 66.003 | 1.00 | 23.52 |
|    | ATOM | 2622 | CA  | GLU | A | 335 | 37.196 | 32.875 | 66.931 | 1.00 | 18.13 |
| 10 | ATOM | 2623 | C   | GLU | A | 335 | 37.278 | 33.384 | 68.346 | 1.00 | 29.15 |
|    | ATOM | 2624 | O   | GLU | A | 335 | 36.357 | 33.124 | 69.112 | 1.00 | 34.14 |
|    | ATOM | 2625 | CB  | GLU | A | 335 | 37.782 | 31.488 | 66.929 | 1.00 | 17.35 |
|    | ATOM | 2626 | CG  | GLU | A | 335 | 37.041 | 30.591 | 67.929 | 1.00 | 32.97 |
|    | ATOM | 2627 | CD  | GLU | A | 335 | 35.642 | 30.305 | 67.473 | 1.00 | 46.14 |
|    | ATOM | 2628 | OE1 | GLU | A | 335 | 35.093 | 30.944 | 66.588 | 1.00 | 39.31 |
| 15 | ATOM | 2629 | OE2 | GLU | A | 335 | 35.080 | 29.317 | 68.132 | 1.00 | 32.80 |
|    | ATOM | 2630 | N   | LYS | A | 336 | 38.370 | 34.077 | 68.706 | 1.00 | 24.53 |
|    | ATOM | 2631 | CA  | LYS | A | 336 | 38.468 | 34.609 | 70.061 | 1.00 | 25.38 |
|    | ATOM | 2632 | C   | LYS | A | 336 | 37.445 | 35.726 | 70.169 | 1.00 | 35.32 |
|    | ATOM | 2633 | O   | LYS | A | 336 | 36.908 | 36.004 | 71.233 | 1.00 | 38.14 |
| 20 | ATOM | 2634 | CB  | LYS | A | 336 | 39.820 | 35.199 | 70.421 | 1.00 | 25.45 |
|    | ATOM | 2635 | CG  | LYS | A | 336 | 40.871 | 34.188 | 70.825 | 1.00 | 25.43 |
|    | ATOM | 2636 | CD  | LYS | A | 336 | 42.207 | 34.846 | 71.189 | 1.00 | 47.10 |
|    | ATOM | 2637 | CE  | LYS | A | 336 | 43.325 | 34.600 | 70.172 | 1.00 | 68.74 |
|    | ATOM | 2638 | NZ  | LYS | A | 336 | 44.566 | 34.072 | 70.767 | 1.00 | 77.62 |
| 25 | ATOM | 2639 | N   | PHE | A | 337 | 37.174 | 36.364 | 69.029 | 1.00 | 31.52 |
|    | ATOM | 2640 | CA  | PHE | A | 337 | 36.186 | 37.442 | 68.967 | 1.00 | 29.34 |
|    | ATOM | 2641 | C   | PHE | A | 337 | 34.783 | 36.869 | 69.083 | 1.00 | 31.73 |
|    | ATOM | 2642 | O   | PHE | A | 337 | 33.908 | 37.424 | 69.742 | 1.00 | 35.53 |
|    | ATOM | 2643 | CB  | PHE | A | 337 | 36.304 | 38.336 | 67.709 | 1.00 | 30.04 |
| 30 | ATOM | 2644 | CG  | PHE | A | 337 | 35.435 | 39.589 | 67.747 | 1.00 | 35.16 |
|    | ATOM | 2645 | CD1 | PHE | A | 337 | 35.468 | 40.459 | 68.843 | 1.00 | 43.88 |
|    | ATOM | 2646 | CD2 | PHE | A | 337 | 34.550 | 39.893 | 66.709 | 1.00 | 40.16 |
|    | ATOM | 2647 | CE1 | PHE | A | 337 | 34.688 | 41.617 | 68.913 | 1.00 | 46.53 |
|    | ATOM | 2648 | CE2 | PHE | A | 337 | 33.753 | 41.040 | 66.760 | 1.00 | 45.62 |
| 35 | ATOM | 2649 | CZ  | PHE | A | 337 | 33.830 | 41.908 | 67.852 | 1.00 | 45.57 |
|    | ATOM | 2650 | N   | ARG | A | 338 | 34.566 | 35.733 | 68.452 | 1.00 | 25.52 |
|    | ATOM | 2651 | CA  | ARG | A | 338 | 33.266 | 35.119 | 68.508 | 1.00 | 25.23 |
|    | ATOM | 2652 | C   | ARG | A | 338 | 32.944 | 34.759 | 69.922 | 1.00 | 29.77 |
|    | ATOM | 2653 | O   | ARG | A | 338 | 31.854 | 35.025 | 70.415 | 1.00 | 31.81 |
| 40 | ATOM | 2654 | CB  | ARG | A | 338 | 33.186 | 33.920 | 67.606 | 1.00 | 24.04 |
|    | ATOM | 2655 | CG  | ARG | A | 338 | 31.839 | 33.228 | 67.623 | 1.00 | 21.31 |
|    | ATOM | 2656 | CD  | ARG | A | 338 | 31.807 | 32.086 | 66.599 | 1.00 | 30.62 |
|    | ATOM | 2657 | NE  | ARG | A | 338 | 32.518 | 30.892 | 67.040 | 1.00 | 29.87 |
|    | ATOM | 2658 | CZ  | ARG | A | 338 | 31.919 | 29.781 | 67.466 | 1.00 | 26.37 |
| 45 | ATOM | 2659 | NH1 | ARG | A | 338 | 30.616 | 29.687 | 67.518 | 1.00 | 20.26 |
|    | ATOM | 2660 | NH2 | ARG | A | 338 | 32.632 | 28.737 | 67.864 | 1.00 | 18.57 |
|    | ATOM | 2661 | N   | HIS | A | 339 | 33.934 | 34.190 | 70.577 | 1.00 | 25.88 |
|    | ATOM | 2662 | CA  | HIS | A | 339 | 33.813 | 33.797 | 71.982 | 1.00 | 25.59 |
|    | ATOM | 2663 | C   | HIS | A | 339 | 33.455 | 34.972 | 72.892 | 1.00 | 27.61 |
| 50 | ATOM | 2664 | O   | HIS | A | 339 | 32.615 | 34.912 | 73.793 | 1.00 | 25.27 |
|    | ATOM | 2665 | CB  | HIS | A | 339 | 35.065 | 33.045 | 72.462 | 1.00 | 25.06 |
|    | ATOM | 2666 | CG  | HIS | A | 339 | 34.923 | 31.587 | 72.155 | 1.00 | 28.13 |
|    | ATOM | 2667 | ND1 | HIS | A | 339 | 35.049 | 30.612 | 73.127 | 1.00 | 30.52 |
|    | ATOM | 2668 | CD2 | HIS | A | 339 | 34.586 | 30.970 | 70.981 | 1.00 | 30.89 |
| 55 | ATOM | 2669 | CE1 | HIS | A | 339 | 34.843 | 29.442 | 72.535 | 1.00 | 30.89 |
|    | ATOM | 2670 | NE2 | HIS | A | 339 | 34.546 | 29.616 | 71.245 | 1.00 | 31.36 |
|    | ATOM | 2671 | N   | PHE | A | 340 | 34.103 | 36.065 | 72.608 | 1.00 | 24.54 |
|    | ATOM | 2672 | CA  | PHE | A | 340 | 33.892 | 37.278 | 73.334 | 1.00 | 25.36 |
|    | ATOM | 2673 | C   | PHE | A | 340 | 32.452 | 37.762 | 73.216 | 1.00 | 32.47 |
| 60 | ATOM | 2674 | O   | PHE | A | 340 | 31.822 | 38.222 | 74.190 | 1.00 | 32.78 |
|    | ATOM | 2675 | CB  | PHE | A | 340 | 34.876 | 38.309 | 72.801 | 1.00 | 26.03 |
|    | ATOM | 2676 | CG  | PHE | A | 340 | 34.654 | 39.671 | 73.346 | 1.00 | 26.47 |
|    | ATOM | 2677 | CD1 | PHE | A | 340 | 35.238 | 40.047 | 74.559 | 1.00 | 24.59 |
|    | ATOM | 2678 | CD2 | PHE | A | 340 | 33.902 | 40.592 | 72.616 | 1.00 | 28.22 |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
|    | ATOM | 2679 | CE1 | PHE | A | 340 | 35.063 | 41.330 | 75.072 | 1.00 | 21.58 |
|    | ATOM | 2680 | CE2 | PHE | A | 340 | 33.715 | 41.879 | 73.115 | 1.00 | 29.13 |
|    | ATOM | 2681 | CZ  | PHE | A | 340 | 34.280 | 42.225 | 74.345 | 1.00 | 25.28 |
| 5  | ATOM | 2682 | N   | ASN | A | 341 | 31.944 | 37.663 | 72.004 | 1.00 | 28.41 |
|    | ATOM | 2683 | CA  | ASN | A | 341 | 30.600 | 38.084 | 71.728 | 1.00 | 29.60 |
|    | ATOM | 2684 | C   | ASN | A | 341 | 29.665 | 37.110 | 72.379 | 1.00 | 38.52 |
|    | ATOM | 2685 | O   | ASN | A | 341 | 28.699 | 37.511 | 73.029 | 1.00 | 42.88 |
|    | ATOM | 2686 | CB  | ASN | A | 341 | 30.322 | 38.274 | 70.224 | 1.00 | 30.01 |
| 10 | ATOM | 2687 | CG  | ASN | A | 341 | 31.159 | 39.374 | 69.587 | 1.00 | 52.80 |
|    | ATOM | 2688 | OD1 | ASN | A | 341 | 31.528 | 39.284 | 68.404 | 1.00 | 60.88 |
|    | ATOM | 2689 | ND2 | ASN | A | 341 | 31.442 | 40.427 | 70.359 | 1.00 | 41.02 |
|    | ATOM | 2690 | N   | ALA | A | 342 | 29.994 | 35.826 | 72.239 | 1.00 | 28.24 |
|    | ATOM | 2691 | CA  | ALA | A | 342 | 29.195 | 34.800 | 72.877 | 1.00 | 26.95 |
|    | ATOM | 2692 | C   | ALA | A | 342 | 29.013 | 35.134 | 74.393 | 1.00 | 35.98 |
| 15 | ATOM | 2693 | O   | ALA | A | 342 | 27.877 | 35.261 | 74.897 | 1.00 | 35.09 |
|    | ATOM | 2694 | CB  | ALA | A | 342 | 29.837 | 33.422 | 72.671 | 1.00 | 25.45 |
|    | ATOM | 2695 | N   | LEU | A | 343 | 30.153 | 35.304 | 75.122 | 1.00 | 29.16 |
|    | ATOM | 2696 | CA  | LEU | A | 343 | 30.162 | 35.633 | 76.560 | 1.00 | 22.58 |
|    | ATOM | 2697 | C   | LEU | A | 343 | 29.310 | 36.854 | 76.831 | 1.00 | 27.48 |
| 20 | ATOM | 2698 | O   | LEU | A | 343 | 28.452 | 36.821 | 77.696 | 1.00 | 32.73 |
|    | ATOM | 2699 | CB  | LEU | A | 343 | 31.583 | 35.786 | 77.147 | 1.00 | 18.70 |
|    | ATOM | 2700 | CG  | LEU | A | 343 | 31.647 | 35.693 | 78.671 | 1.00 | 20.08 |
|    | ATOM | 2701 | CD1 | LEU | A | 343 | 30.842 | 34.510 | 79.204 | 1.00 | 17.76 |
|    | ATOM | 2702 | CD2 | LEU | A | 343 | 33.091 | 35.522 | 79.111 | 1.00 | 21.94 |
| 25 | ATOM | 2703 | N   | GLY | A | 344 | 29.512 | 37.936 | 76.080 | 1.00 | 22.60 |
|    | ATOM | 2704 | CA  | GLY | A | 344 | 28.670 | 39.146 | 76.278 | 1.00 | 24.15 |
|    | ATOM | 2705 | C   | GLY | A | 344 | 27.157 | 38.824 | 76.136 | 1.00 | 31.38 |
|    | ATOM | 2706 | O   | GLY | A | 344 | 26.339 | 39.260 | 76.943 | 1.00 | 32.44 |
|    | ATOM | 2707 | N   | GLY | A | 345 | 26.806 | 38.017 | 75.094 | 1.00 | 22.79 |
| 30 | ATOM | 2708 | CA  | GLY | A | 345 | 25.451 | 37.587 | 74.801 | 1.00 | 19.88 |
|    | ATOM | 2709 | C   | GLY | A | 345 | 24.787 | 36.994 | 76.034 | 1.00 | 28.37 |
|    | ATOM | 2710 | O   | GLY | A | 345 | 23.632 | 37.294 | 76.325 | 1.00 | 27.56 |
|    | ATOM | 2711 | N   | TRP | A | 346 | 25.547 | 36.153 | 76.765 | 1.00 | 25.41 |
|    | ATOM | 2712 | CA  | TRP | A | 346 | 25.082 | 35.520 | 77.994 | 1.00 | 23.90 |
| 35 | ATOM | 2713 | C   | TRP | A | 346 | 24.825 | 36.541 | 79.071 | 1.00 | 31.54 |
|    | ATOM | 2714 | O   | TRP | A | 346 | 23.957 | 36.379 | 79.924 | 1.00 | 29.57 |
|    | ATOM | 2715 | CB  | TRP | A | 346 | 26.122 | 34.556 | 78.562 | 1.00 | 21.53 |
|    | ATOM | 2716 | CG  | TRP | A | 346 | 25.680 | 33.880 | 79.837 | 1.00 | 21.92 |
|    | ATOM | 2717 | CD1 | TRP | A | 346 | 25.933 | 34.335 | 81.079 | 1.00 | 24.36 |
| 40 | ATOM | 2718 | CD2 | TRP | A | 346 | 25.004 | 32.597 | 80.010 | 1.00 | 20.97 |
|    | ATOM | 2719 | NE1 | TRP | A | 346 | 25.450 | 33.453 | 82.008 | 1.00 | 23.95 |
|    | ATOM | 2720 | CE2 | TRP | A | 346 | 24.859 | 32.388 | 81.391 | 1.00 | 24.13 |
|    | ATOM | 2721 | CE3 | TRP | A | 346 | 24.488 | 31.611 | 79.144 | 1.00 | 21.46 |
|    | ATOM | 2722 | CZ2 | TRP | A | 346 | 24.225 | 31.244 | 81.921 | 1.00 | 22.89 |
| 45 | ATOM | 2723 | CZ3 | TRP | A | 346 | 23.872 | 30.477 | 79.662 | 1.00 | 22.03 |
|    | ATOM | 2724 | CH2 | TRP | A | 346 | 23.747 | 30.286 | 81.046 | 1.00 | 21.87 |
|    | ATOM | 2725 | N   | GLY | A | 347 | 25.627 | 37.593 | 79.039 | 1.00 | 29.66 |
|    | ATOM | 2726 | CA  | GLY | A | 347 | 25.465 | 38.625 | 80.042 | 1.00 | 29.03 |
|    | ATOM | 2727 | C   | GLY | A | 347 | 24.156 | 39.333 | 79.844 | 1.00 | 33.01 |
| 50 | ATOM | 2728 | O   | GLY | A | 347 | 23.491 | 39.647 | 80.799 | 1.00 | 34.17 |
|    | ATOM | 2729 | N   | GLU | A | 348 | 23.797 | 39.574 | 78.581 | 1.00 | 30.57 |
|    | ATOM | 2730 | CA  | GLU | A | 348 | 22.535 | 40.220 | 78.250 | 1.00 | 29.17 |
|    | ATOM | 2731 | C   | GLU | A | 348 | 21.423 | 39.282 | 78.664 | 1.00 | 31.25 |
|    | ATOM | 2732 | O   | GLU | A | 348 | 20.373 | 39.663 | 79.142 | 1.00 | 33.71 |
| 55 | ATOM | 2733 | CB  | GLU | A | 348 | 22.432 | 40.606 | 76.757 | 1.00 | 30.33 |
|    | ATOM | 2734 | CG  | GLU | A | 348 | 23.432 | 41.715 | 76.336 | 1.00 | 49.41 |
|    | ATOM | 2735 | CD  | GLU | A | 348 | 23.209 | 43.088 | 76.964 | 1.00 | 73.39 |
|    | ATOM | 2736 | OE1 | GLU | A | 348 | 22.295 | 43.846 | 76.656 | 1.00 | 71.22 |
|    | ATOM | 2737 | OE2 | GLU | A | 348 | 24.119 | 43.395 | 77.857 | 1.00 | 44.23 |
| 60 | ATOM | 2738 | N   | LEU | A | 349 | 21.682 | 38.011 | 78.541 | 1.00 | 27.36 |
|    | ATOM | 2739 | CA  | LEU | A | 349 | 20.677 | 37.081 | 78.976 | 1.00 | 26.89 |
|    | ATOM | 2740 | C   | LEU | A | 349 | 20.429 | 37.250 | 80.485 | 1.00 | 24.87 |
|    | ATOM | 2741 | O   | LEU | A | 349 | 19.299 | 37.403 | 80.914 | 1.00 | 28.31 |
|    | ATOM | 2742 | CB  | LEU | A | 349 | 20.984 | 35.630 | 78.529 | 1.00 | 27.18 |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
|    | ATOM | 2743 | CG  | LEU | A | 349 | 19.943 | 34.565 | 78.942 | 1.00 | 32.45 |
|    | ATOM | 2744 | CD1 | LEU | A | 349 | 18.611 | 34.704 | 78.154 | 1.00 | 30.09 |
|    | ATOM | 2745 | CD2 | LEU | A | 349 | 20.541 | 33.169 | 78.749 | 1.00 | 27.10 |
| 5  | ATOM | 2746 | N   | GLN | A | 350 | 21.460 | 37.255 | 81.315 | 1.00 | 14.78 |
|    | ATOM | 2747 | CA  | GLN | A | 350 | 21.188 | 37.428 | 82.727 | 1.00 | 18.51 |
|    | ATOM | 2748 | C   | GLN | A | 350 | 20.442 | 38.722 | 82.953 | 1.00 | 25.53 |
|    | ATOM | 2749 | O   | GLN | A | 350 | 19.495 | 38.833 | 83.737 | 1.00 | 28.35 |
|    | ATOM | 2750 | CB  | GLN | A | 350 | 22.469 | 37.369 | 83.536 | 1.00 | 22.22 |
| 10 | ATOM | 2751 | CG  | GLN | A | 350 | 23.512 | 36.426 | 82.919 | 1.00 | 22.37 |
|    | ATOM | 2752 | CD  | GLN | A | 350 | 24.871 | 36.673 | 83.547 | 1.00 | 34.49 |
|    | ATOM | 2753 | OE1 | GLN | A | 350 | 25.261 | 35.932 | 84.417 | 1.00 | 24.01 |
|    | ATOM | 2754 | NE2 | GLN | A | 350 | 25.588 | 37.727 | 83.127 | 1.00 | 36.58 |
|    | ATOM | 2755 | N   | ASN | A | 351 | 20.838 | 39.696 | 82.201 | 1.00 | 22.64 |
|    | ATOM | 2756 | CA  | ASN | A | 351 | 20.163 | 40.960 | 82.273 | 1.00 | 26.10 |
| 15 | ATOM | 2757 | C   | ASN | A | 351 | 18.661 | 40.780 | 82.083 | 1.00 | 37.49 |
|    | ATOM | 2758 | O   | ASN | A | 351 | 17.890 | 41.098 | 82.977 | 1.00 | 41.41 |
|    | ATOM | 2759 | CB  | ASN | A | 351 | 20.769 | 42.021 | 81.341 | 1.00 | 20.74 |
|    | ATOM | 2760 | CG  | ASN | A | 351 | 22.118 | 42.477 | 81.847 | 1.00 | 23.25 |
| 20 | ATOM | 2761 | OD1 | ASN | A | 351 | 22.692 | 41.875 | 82.771 | 1.00 | 26.88 |
|    | ATOM | 2762 | ND2 | ASN | A | 351 | 22.644 | 43.530 | 81.247 | 1.00 | 32.93 |
|    | ATOM | 2763 | N   | SER | A | 352 | 18.228 | 40.252 | 80.938 | 1.00 | 32.84 |
|    | ATOM | 2764 | CA  | SER | A | 352 | 16.784 | 40.041 | 80.715 | 1.00 | 34.27 |
|    | ATOM | 2765 | C   | SER | A | 352 | 16.107 | 39.135 | 81.784 | 1.00 | 31.72 |
| 25 | ATOM | 2766 | O   | SER | A | 352 | 14.927 | 39.266 | 82.189 | 1.00 | 28.64 |
|    | ATOM | 2767 | CB  | SER | A | 352 | 16.503 | 39.531 | 79.301 | 1.00 | 42.57 |
|    | ATOM | 2768 | OG  | SER | A | 352 | 17.506 | 39.979 | 78.407 | 1.00 | 49.17 |
|    | ATOM | 2769 | N   | VAL | A | 353 | 16.874 | 38.188 | 82.247 | 1.00 | 21.90 |
|    | ATOM | 2770 | CA  | VAL | A | 353 | 16.322 | 37.351 | 83.234 | 1.00 | 22.13 |
| 30 | ATOM | 2771 | C   | VAL | A | 353 | 16.068 | 38.122 | 84.516 | 1.00 | 36.22 |
|    | ATOM | 2772 | O   | VAL | A | 353 | 14.958 | 38.076 | 85.052 | 1.00 | 37.69 |
|    | ATOM | 2773 | CB  | VAL | A | 353 | 17.137 | 36.070 | 83.419 | 1.00 | 20.84 |
|    | ATOM | 2774 | CG1 | VAL | A | 353 | 16.632 | 35.256 | 84.634 | 1.00 | 15.06 |
|    | ATOM | 2775 | CG2 | VAL | A | 353 | 16.968 | 35.284 | 82.105 | 1.00 | 20.93 |
| 35 | ATOM | 2776 | N   | LYS | A | 354 | 17.086 | 38.847 | 85.002 | 1.00 | 30.67 |
|    | ATOM | 2777 | CA  | LYS | A | 354 | 16.880 | 39.587 | 86.221 | 1.00 | 31.71 |
|    | ATOM | 2778 | C   | LYS | A | 354 | 15.660 | 40.474 | 86.098 | 1.00 | 36.17 |
|    | ATOM | 2779 | O   | LYS | A | 354 | 14.808 | 40.582 | 86.980 | 1.00 | 35.80 |
|    | ATOM | 2780 | CB  | LYS | A | 354 | 18.099 | 40.396 | 86.624 | 1.00 | 35.28 |
| 40 | ATOM | 2781 | CG  | LYS | A | 354 | 17.841 | 41.303 | 87.818 | 1.00 | 51.51 |
|    | ATOM | 2782 | CD  | LYS | A | 354 | 19.038 | 41.405 | 88.749 | 1.00 | 60.46 |
|    | ATOM | 2783 | CE  | LYS | A | 354 | 19.198 | 42.780 | 89.383 | 1.00 | 50.09 |
|    | ATOM | 2784 | NZ  | LYS | A | 354 | 20.596 | 43.133 | 89.657 | 1.00 | 63.77 |
|    | ATOM | 2785 | N   | THR | A | 355 | 15.608 | 41.108 | 84.962 | 1.00 | 32.63 |
| 45 | ATOM | 2786 | CA  | THR | A | 355 | 14.562 | 42.025 | 84.610 | 1.00 | 34.03 |
|    | ATOM | 2787 | C   | THR | A | 355 | 13.129 | 41.422 | 84.578 | 1.00 | 42.11 |
|    | ATOM | 2788 | O   | THR | A | 355 | 12.216 | 42.006 | 85.154 | 1.00 | 40.96 |
|    | ATOM | 2789 | CB  | THR | A | 355 | 14.974 | 42.736 | 83.308 | 1.00 | 41.11 |
|    | ATOM | 2790 | OG1 | THR | A | 355 | 16.071 | 43.615 | 83.542 | 1.00 | 29.85 |
| 50 | ATOM | 2791 | CG2 | THR | A | 355 | 13.798 | 43.438 | 82.656 | 1.00 | 45.50 |
|    | ATOM | 2792 | N   | PHE | A | 356 | 12.895 | 40.273 | 83.908 | 1.00 | 33.89 |
|    | ATOM | 2793 | CA  | PHE | A | 356 | 11.556 | 39.729 | 83.860 | 1.00 | 29.29 |
|    | ATOM | 2794 | C   | PHE | A | 356 | 11.209 | 39.070 | 85.147 | 1.00 | 31.93 |
|    | ATOM | 2795 | O   | PHE | A | 356 | 10.089 | 39.152 | 85.642 | 1.00 | 33.85 |
| 55 | ATOM | 2796 | CB  | PHE | A | 356 | 11.460 | 38.645 | 82.785 | 1.00 | 33.30 |
|    | ATOM | 2797 | CG  | PHE | A | 356 | 11.187 | 39.196 | 81.416 | 1.00 | 36.54 |
|    | ATOM | 2798 | CD1 | PHE | A | 356 | 10.106 | 40.054 | 81.224 | 1.00 | 42.38 |
|    | ATOM | 2799 | CD2 | PHE | A | 356 | 11.985 | 38.858 | 80.320 | 1.00 | 38.62 |
|    | ATOM | 2800 | CE1 | PHE | A | 356 | 9.831  | 40.596 | 79.968 | 1.00 | 44.75 |
|    | ATOM | 2801 | CE2 | PHE | A | 356 | 11.723 | 39.384 | 79.055 | 1.00 | 43.46 |
| 60 | ATOM | 2802 | CZ  | PHE | A | 356 | 10.649 | 40.261 | 78.890 | 1.00 | 43.86 |
|    | ATOM | 2803 | N   | GLY | A | 357 | 12.212 | 38.386 | 85.661 | 1.00 | 30.41 |
|    | ATOM | 2804 | CA  | GLY | A | 357 | 12.152 | 37.564 | 86.864 | 1.00 | 29.17 |
|    | ATOM | 2805 | C   | GLY | A | 357 | 12.446 | 36.100 | 86.438 | 1.00 | 28.92 |
|    | ATOM | 2806 | O   | GLY | A | 357 | 12.008 | 35.642 | 85.372 | 1.00 | 27.33 |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
|    | ATOM | 2807 | N   | GLU | A | 358 | 13.211 | 35.382 | 87.243 | 1.00 | 21.27 |
|    | ATOM | 2808 | CA  | GLU | A | 358 | 13.590 | 34.040 | 86.898 | 1.00 | 23.10 |
|    | ATOM | 2809 | C   | GLU | A | 358 | 12.424 | 33.104 | 86.747 | 1.00 | 31.53 |
| 5  | ATOM | 2810 | O   | GLU | A | 358 | 12.581 | 31.972 | 86.294 | 1.00 | 30.92 |
|    | ATOM | 2811 | CB  | GLU | A | 358 | 14.596 | 33.473 | 87.880 | 1.00 | 25.36 |
|    | ATOM | 2812 | CG  | GLU | A | 358 | 14.011 | 33.436 | 89.301 | 1.00 | 38.73 |
|    | ATOM | 2813 | CD  | GLU | A | 358 | 15.011 | 33.037 | 90.345 | 1.00 | 56.34 |
|    | ATOM | 2814 | OE1 | GLU | A | 358 | 16.026 | 32.446 | 90.071 | 1.00 | 50.55 |
| 10 | ATOM | 2815 | OE2 | GLU | A | 358 | 14.678 | 33.403 | 91.564 | 1.00 | 75.65 |
|    | ATOM | 2816 | N   | THR | A | 359 | 11.246 | 33.542 | 87.139 | 1.00 | 27.87 |
|    | ATOM | 2817 | CA  | THR | A | 359 | 10.154 | 32.625 | 86.970 | 1.00 | 25.66 |
|    | ATOM | 2818 | C   | THR | A | 359 | 9.236  | 33.152 | 85.906 | 1.00 | 25.96 |
|    | ATOM | 2819 | O   | THR | A | 359 | 8.247  | 32.528 | 85.533 | 1.00 | 25.58 |
| 15 | ATOM | 2820 | CB  | THR | A | 359 | 9.423  | 32.341 | 88.253 | 1.00 | 25.00 |
|    | ATOM | 2821 | OG1 | THR | A | 359 | 8.908  | 33.565 | 88.692 | 1.00 | 33.10 |
|    | ATOM | 2822 | CG2 | THR | A | 359 | 10.406 | 31.785 | 89.273 | 1.00 | 14.43 |
|    | ATOM | 2823 | N   | HIS | A | 360 | 9.602  | 34.310 | 85.407 | 1.00 | 20.75 |
|    | ATOM | 2824 | CA  | HIS | A | 360 | 8.837  | 34.902 | 84.363 | 1.00 | 22.77 |
| 20 | ATOM | 2825 | C   | HIS | A | 360 | 8.823  | 34.034 | 83.130 | 1.00 | 35.30 |
|    | ATOM | 2826 | O   | HIS | A | 360 | 9.858  | 33.611 | 82.620 | 1.00 | 37.42 |
|    | ATOM | 2827 | CB  | HIS | A | 360 | 9.294  | 36.291 | 83.982 | 1.00 | 23.18 |
|    | ATOM | 2828 | CG  | HIS | A | 360 | 8.207  | 36.908 | 83.219 | 1.00 | 27.05 |
|    | ATOM | 2829 | ND1 | HIS | A | 360 | 7.532  | 38.009 | 83.691 | 1.00 | 29.34 |
| 25 | ATOM | 2830 | CD2 | HIS | A | 360 | 7.651  | 36.545 | 82.059 | 1.00 | 29.91 |
|    | ATOM | 2831 | CE1 | HIS | A | 360 | 6.596  | 38.315 | 82.806 | 1.00 | 27.94 |
|    | ATOM | 2832 | NE2 | HIS | A | 360 | 6.651  | 37.440 | 81.812 | 1.00 | 29.60 |
|    | ATOM | 2833 | N   | PRO | A | 361 | 7.606  | 33.817 | 82.666 | 1.00 | 32.40 |
|    | ATOM | 2834 | CA  | PRO | A | 361 | 7.301  | 32.999 | 81.519 | 1.00 | 29.46 |
| 30 | ATOM | 2835 | C   | PRO | A | 361 | 7.862  | 33.478 | 80.224 | 1.00 | 30.59 |
|    | ATOM | 2836 | O   | PRO | A | 361 | 7.907  | 32.737 | 79.248 | 1.00 | 33.00 |
|    | ATOM | 2837 | CB  | PRO | A | 361 | 5.770  | 32.963 | 81.478 | 1.00 | 30.74 |
|    | ATOM | 2838 | CG  | PRO | A | 361 | 5.311  | 33.172 | 82.927 | 1.00 | 34.96 |
|    | ATOM | 2839 | CD  | PRO | A | 361 | 6.463  | 33.869 | 83.627 | 1.00 | 31.82 |
| 35 | ATOM | 2840 | N   | PHE | A | 362 | 8.289  | 34.712 | 80.179 | 1.00 | 26.32 |
|    | ATOM | 2841 | CA  | PHE | A | 362 | 8.823  | 35.173 | 78.933 | 1.00 | 25.68 |
|    | ATOM | 2842 | C   | PHE | A | 362 | 10.261 | 34.781 | 78.829 | 1.00 | 29.73 |
|    | ATOM | 2843 | O   | PHE | A | 362 | 10.906 | 35.131 | 77.870 | 1.00 | 32.02 |
|    | ATOM | 2844 | CB  | PHE | A | 362 | 8.643  | 36.677 | 78.723 | 1.00 | 28.12 |
| 40 | ATOM | 2845 | CG  | PHE | A | 362 | 7.194  | 37.105 | 78.629 | 1.00 | 30.03 |
|    | ATOM | 2846 | CD1 | PHE | A | 362 | 6.204  | 36.276 | 78.098 | 1.00 | 30.92 |
|    | ATOM | 2847 | CD2 | PHE | A | 362 | 6.804  | 38.372 | 79.051 | 1.00 | 32.04 |
|    | ATOM | 2848 | CE1 | PHE | A | 362 | 4.864  | 36.655 | 77.998 | 1.00 | 26.59 |
|    | ATOM | 2849 | CE2 | PHE | A | 362 | 5.470  | 38.773 | 78.952 | 1.00 | 32.40 |
| 45 | ATOM | 2850 | CZ  | PHE | A | 362 | 4.495  | 37.920 | 78.435 | 1.00 | 26.37 |
|    | ATOM | 2851 | N   | THR | A | 363 | 10.730 | 34.049 | 79.843 | 1.00 | 27.22 |
|    | ATOM | 2852 | CA  | THR | A | 363 | 12.102 | 33.575 | 79.943 | 1.00 | 27.52 |
|    | ATOM | 2853 | C   | THR | A | 363 | 12.251 | 32.132 | 79.504 | 1.00 | 29.28 |
|    | ATOM | 2854 | O   | THR | A | 363 | 13.331 | 31.560 | 79.524 | 1.00 | 29.42 |
| 50 | ATOM | 2855 | CB  | THR | A | 363 | 12.697 | 33.777 | 81.360 | 1.00 | 31.67 |
|    | ATOM | 2856 | OG1 | THR | A | 363 | 12.279 | 32.745 | 82.218 | 1.00 | 26.17 |
|    | ATOM | 2857 | CG2 | THR | A | 363 | 12.278 | 35.118 | 81.930 | 1.00 | 31.62 |
|    | ATOM | 2858 | N   | LYS | A | 364 | 11.148 | 31.530 | 79.113 | 1.00 | 23.08 |
|    | ATOM | 2859 | CA  | LYS | A | 364 | 11.174 | 30.160 | 78.664 | 1.00 | 20.50 |
| 55 | ATOM | 2860 | C   | LYS | A | 364 | 11.556 | 30.270 | 77.217 | 1.00 | 28.83 |
|    | ATOM | 2861 | O   | LYS | A | 364 | 11.139 | 31.239 | 76.570 | 1.00 | 29.80 |
|    | ATOM | 2862 | CB  | LYS | A | 364 | 9.766  | 29.584 | 78.667 | 1.00 | 23.55 |
|    | ATOM | 2863 | CG  | LYS | A | 364 | 9.252  | 29.134 | 80.022 | 1.00 | 40.85 |
|    | ATOM | 2864 | CD  | LYS | A | 364 | 7.761  | 29.369 | 80.162 | 1.00 | 44.83 |
| 60 | ATOM | 2865 | CE  | LYS | A | 364 | 7.131  | 28.492 | 81.224 | 1.00 | 66.38 |
|    | ATOM | 2866 | NZ  | LYS | A | 364 | 6.063  | 27.638 | 80.691 | 1.00 | 91.70 |
|    | ATOM | 2867 | N   | LEU | A | 365 | 12.332 | 29.328 | 76.698 | 1.00 | 23.57 |
|    | ATOM | 2868 | CA  | LEU | A | 365 | 12.699 | 29.420 | 75.312 | 1.00 | 23.95 |
|    | ATOM | 2869 | C   | LEU | A | 365 | 11.414 | 29.419 | 74.445 | 1.00 | 35.57 |
|    | ATOM | 2870 | O   | LEU | A | 365 | 11.166 | 30.369 | 73.708 | 1.00 | 34.58 |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5  | ATOM | 2871 | CB  | LEU | A | 365 | 13.702 | 28.303 | 75.021 | 1.00 | 25.08 |
|    | ATOM | 2872 | CG  | LEU | A | 365 | 14.456 | 28.372 | 73.702 | 1.00 | 31.15 |
|    | ATOM | 2873 | CD1 | LEU | A | 365 | 14.987 | 29.778 | 73.466 | 1.00 | 33.16 |
|    | ATOM | 2874 | CD2 | LEU | A | 365 | 15.609 | 27.353 | 73.781 | 1.00 | 30.62 |
|    | ATOM | 2875 | N   | VAL | A | 366 | 10.572 | 28.360 | 74.564 | 1.00 | 35.62 |
| 10 | ATOM | 2876 | CA  | VAL | A | 366 | 9.294  | 28.232 | 73.840 | 1.00 | 32.10 |
|    | ATOM | 2877 | C   | VAL | A | 366 | 8.211  | 28.911 | 74.694 | 1.00 | 33.14 |
|    | ATOM | 2878 | O   | VAL | A | 366 | 7.982  | 28.470 | 75.808 | 1.00 | 34.20 |
|    | ATOM | 2879 | CB  | VAL | A | 366 | 8.936  | 26.739 | 73.568 | 1.00 | 34.73 |
|    | ATOM | 2880 | CG1 | VAL | A | 366 | 7.558  | 26.605 | 72.933 | 1.00 | 34.88 |
| 15 | ATOM | 2881 | CG2 | VAL | A | 366 | 9.922  | 26.012 | 72.649 | 1.00 | 32.65 |
|    | ATOM | 2882 | N   | VAL | A | 367 | 7.562  | 29.990 | 74.211 | 1.00 | 28.76 |
|    | ATOM | 2883 | CA  | VAL | A | 367 | 6.532  | 30.700 | 74.987 | 1.00 | 28.27 |
|    | ATOM | 2884 | C   | VAL | A | 367 | 5.161  | 30.613 | 74.420 | 1.00 | 30.62 |
|    | ATOM | 2885 | O   | VAL | A | 367 | 4.994  | 30.509 | 73.235 | 1.00 | 34.30 |
| 20 | ATOM | 2886 | CB  | VAL | A | 367 | 6.773  | 32.185 | 75.061 | 1.00 | 33.45 |
|    | ATOM | 2887 | CG1 | VAL | A | 367 | 8.178  | 32.478 | 75.565 | 1.00 | 33.03 |
|    | ATOM | 2888 | CG2 | VAL | A | 367 | 6.498  | 32.804 | 73.693 | 1.00 | 33.18 |
|    | ATOM | 2889 | N   | ASP | A | 368 | 4.168  | 30.722 | 75.290 | 1.00 | 29.27 |
|    | ATOM | 2890 | CA  | ASP | A | 368 | 2.764  | 30.771 | 74.984 | 1.00 | 27.67 |
| 25 | ATOM | 2891 | C   | ASP | A | 368 | 2.315  | 32.207 | 74.862 | 1.00 | 26.94 |
|    | ATOM | 2892 | O   | ASP | A | 368 | 2.283  | 32.975 | 75.830 | 1.00 | 23.11 |
|    | ATOM | 2893 | CB  | ASP | A | 368 | 1.990  | 30.073 | 76.100 | 1.00 | 26.80 |
|    | ATOM | 2894 | CG  | ASP | A | 368 | 0.572  | 29.781 | 75.613 | 1.00 | 37.90 |
|    | ATOM | 2895 | OD1 | ASP | A | 368 | 0.276  | 30.123 | 74.481 | 1.00 | 38.93 |
| 30 | ATOM | 2896 | OD2 | ASP | A | 368 | -0.215 | 29.217 | 76.380 | 1.00 | 38.59 |
|    | ATOM | 2897 | N   | LEU | A | 369 | 2.027  | 32.588 | 73.622 | 1.00 | 26.55 |
|    | ATOM | 2898 | CA  | LEU | A | 369 | 1.643  | 33.953 | 73.373 | 1.00 | 27.39 |
|    | ATOM | 2899 | C   | LEU | A | 369 | 0.138  | 34.105 | 73.301 | 1.00 | 30.74 |
|    | ATOM | 2900 | O   | LEU | A | 369 | -0.372 | 34.979 | 72.648 | 1.00 | 30.68 |
| 35 | ATOM | 2901 | CB  | LEU | A | 369 | 2.281  | 34.395 | 72.064 | 1.00 | 26.06 |
|    | ATOM | 2902 | CG  | LEU | A | 369 | 3.759  | 34.760 | 72.229 | 1.00 | 26.80 |
|    | ATOM | 2903 | CD1 | LEU | A | 369 | 4.343  | 35.415 | 70.994 | 1.00 | 24.30 |
|    | ATOM | 2904 | CD2 | LEU | A | 369 | 4.014  | 35.728 | 73.384 | 1.00 | 21.81 |
|    | ATOM | 2905 | N   | THR | A | 370 | -0.577 | 33.154 | 73.953 | 1.00 | 30.26 |
| 40 | ATOM | 2906 | CA  | THR | A | 370 | -2.022 | 33.306 | 74.093 | 1.00 | 31.38 |
|    | ATOM | 2907 | C   | THR | A | 370 | -2.355 | 34.519 | 74.941 | 1.00 | 38.62 |
|    | ATOM | 2908 | O   | THR | A | 370 | -1.821 | 34.714 | 76.027 | 1.00 | 38.84 |
|    | ATOM | 2909 | CB  | THR | A | 370 | -2.601 | 32.056 | 74.750 | 1.00 | 34.04 |
|    | ATOM | 2910 | OG1 | THR | A | 370 | -2.472 | 30.949 | 73.873 | 1.00 | 29.99 |
| 45 | ATOM | 2911 | CG2 | THR | A | 370 | -4.091 | 32.266 | 75.052 | 1.00 | 26.40 |
|    | ATOM | 2912 | N   | ASP | A | 371 | -3.173 | 35.387 | 74.363 | 1.00 | 37.89 |
|    | ATOM | 2913 | CA  | ASP | A | 371 | -3.641 | 36.612 | 75.012 | 1.00 | 37.85 |
|    | ATOM | 2914 | C   | ASP | A | 371 | -2.557 | 37.636 | 75.255 | 1.00 | 40.92 |
|    | ATOM | 2915 | O   | ASP | A | 371 | -2.784 | 38.625 | 75.933 | 1.00 | 41.63 |
| 50 | ATOM | 2916 | CB  | ASP | A | 371 | -4.519 | 36.375 | 76.245 | 1.00 | 39.88 |
|    | ATOM | 2917 | CG  | ASP | A | 371 | -5.805 | 35.733 | 75.798 | 1.00 | 51.30 |
|    | ATOM | 2918 | OD1 | ASP | A | 371 | -6.373 | 36.072 | 74.761 | 1.00 | 50.39 |
|    | ATOM | 2919 | OD2 | ASP | A | 371 | -6.206 | 34.754 | 76.583 | 1.00 | 48.61 |
|    | ATOM | 2920 | N   | ILE | A | 372 | -1.387 | 37.398 | 74.664 | 1.00 | 36.37 |
| 55 | ATOM | 2921 | CA  | ILE | A | 372 | -0.259 | 38.283 | 74.817 | 1.00 | 34.61 |
|    | ATOM | 2922 | C   | ILE | A | 372 | 0.203  | 39.018 | 73.555 | 1.00 | 35.46 |
|    | ATOM | 2923 | O   | ILE | A | 372 | 0.545  | 38.400 | 72.548 | 1.00 | 36.69 |
|    | ATOM | 2924 | CB  | ILE | A | 372 | 0.920  | 37.511 | 75.381 | 1.00 | 36.51 |
|    | ATOM | 2925 | CG1 | ILE | A | 372 | 0.658  | 37.195 | 76.842 | 1.00 | 37.01 |
| 60 | ATOM | 2926 | CG2 | ILE | A | 372 | 2.121  | 38.441 | 75.281 | 1.00 | 35.52 |
|    | ATOM | 2927 | CD1 | ILE | A | 372 | 1.268  | 38.261 | 77.747 | 1.00 | 54.33 |
|    | ATOM | 2928 | N   | ASP | A | 373 | 0.254  | 40.345 | 73.601 | 1.00 | 25.92 |
|    | ATOM | 2929 | CA  | ASP | A | 373 | 0.747  | 41.053 | 72.450 | 1.00 | 23.77 |
|    | ATOM | 2930 | C   | ASP | A | 373 | 2.263  | 40.781 | 72.360 | 1.00 | 31.40 |
|    | ATOM | 2931 | O   | ASP | A | 373 | 3.040  | 41.002 | 73.305 | 1.00 | 32.80 |
|    | ATOM | 2932 | CB  | ASP | A | 373 | 0.408  | 42.543 | 72.519 | 1.00 | 25.08 |
|    | ATOM | 2933 | CG  | ASP | A | 373 | 1.064  | 43.356 | 71.418 | 1.00 | 43.24 |
|    | ATOM | 2934 | OD1 | ASP | A | 373 | 1.861  | 42.894 | 70.616 | 1.00 | 45.30 |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5  | ATOM | 2935 | OD2 | ASP | A | 373 | 0.668  | 44.610 | 71.395 | 1.00 | 38.59 |
|    | ATOM | 2936 | N   | PRO | A | 374 | 2.709  | 40.267 | 71.225 | 1.00 | 29.51 |
|    | ATOM | 2937 | CA  | PRO | A | 374 | 4.123  | 39.943 | 71.132 | 1.00 | 28.52 |
|    | ATOM | 2938 | C   | PRO | A | 374 | 5.029  | 41.090 | 71.506 | 1.00 | 32.54 |
|    | ATOM | 2939 | O   | PRO | A | 374 | 6.019  | 40.905 | 72.217 | 1.00 | 29.62 |
| 10 | ATOM | 2940 | CB  | PRO | A | 374 | 4.390  | 39.421 | 69.714 | 1.00 | 28.88 |
|    | ATOM | 2941 | CG  | PRO | A | 374 | 3.028  | 39.278 | 69.032 | 1.00 | 32.27 |
|    | ATOM | 2942 | CD  | PRO | A | 374 | 1.966  | 39.786 | 70.008 | 1.00 | 28.84 |
|    | ATOM | 2943 | N   | ASP | A | 375 | 4.660  | 42.257 | 70.981 | 1.00 | 26.85 |
|    | ATOM | 2944 | CA  | ASP | A | 375 | 5.357  | 43.511 | 71.154 | 1.00 | 24.25 |
| 15 | ATOM | 2945 | C   | ASP | A | 375 | 5.695  | 43.783 | 72.628 | 1.00 | 33.10 |
|    | ATOM | 2946 | O   | ASP | A | 375 | 6.648  | 44.494 | 72.988 | 1.00 | 30.67 |
|    | ATOM | 2947 | CB  | ASP | A | 375 | 4.507  | 44.617 | 70.509 | 1.00 | 24.46 |
|    | ATOM | 2948 | CG  | ASP | A | 375 | 4.753  | 44.836 | 69.033 | 1.00 | 30.08 |
|    | ATOM | 2949 | OD1 | ASP | A | 375 | 5.703  | 44.393 | 68.411 | 1.00 | 33.47 |
| 20 | ATOM | 2950 | OD2 | ASP | A | 375 | 3.852  | 45.609 | 68.491 | 1.00 | 38.41 |
|    | ATOM | 2951 | N   | VAL | A | 376 | 4.885  | 43.161 | 73.477 | 1.00 | 30.21 |
|    | ATOM | 2952 | CA  | VAL | A | 376 | 5.001  | 43.232 | 74.904 | 1.00 | 25.40 |
|    | ATOM | 2953 | C   | VAL | A | 376 | 5.879  | 42.106 | 75.431 | 1.00 | 37.27 |
|    | ATOM | 2954 | O   | VAL | A | 376 | 6.599  | 42.299 | 76.394 | 1.00 | 42.46 |
| 25 | ATOM | 2955 | CB  | VAL | A | 376 | 3.638  | 43.099 | 75.550 | 1.00 | 22.48 |
|    | ATOM | 2956 | CG1 | VAL | A | 376 | 3.799  | 42.533 | 76.975 | 1.00 | 21.25 |
|    | ATOM | 2957 | CG2 | VAL | A | 376 | 2.926  | 44.440 | 75.547 | 1.00 | 18.29 |
|    | ATOM | 2958 | N   | ALA | A | 377 | 5.811  | 40.905 | 74.831 | 1.00 | 30.48 |
|    | ATOM | 2959 | CA  | ALA | A | 377 | 6.671  | 39.793 | 75.288 | 1.00 | 27.04 |
| 30 | ATOM | 2960 | C   | ALA | A | 377 | 8.149  | 39.911 | 74.797 | 1.00 | 28.15 |
|    | ATOM | 2961 | O   | ALA | A | 377 | 9.077  | 39.325 | 75.312 | 1.00 | 27.36 |
|    | ATOM | 2962 | CB  | ALA | A | 377 | 6.091  | 38.433 | 74.891 | 1.00 | 26.74 |
|    | ATOM | 2963 | N   | TYR | A | 378 | 8.376  | 40.692 | 73.768 | 1.00 | 25.81 |
|    | ATOM | 2964 | CA  | TYR | A | 378 | 9.683  | 40.876 | 73.161 | 1.00 | 25.43 |
| 35 | ATOM | 2965 | C   | TYR | A | 378 | 10.862 | 41.194 | 74.057 | 1.00 | 30.49 |
|    | ATOM | 2966 | O   | TYR | A | 378 | 10.873 | 42.204 | 74.747 | 1.00 | 32.35 |
|    | ATOM | 2967 | CB  | TYR | A | 378 | 9.549  | 41.924 | 72.068 | 1.00 | 26.20 |
|    | ATOM | 2968 | CG  | TYR | A | 378 | 10.804 | 42.168 | 71.327 | 1.00 | 19.90 |
|    | ATOM | 2969 | CD1 | TYR | A | 378 | 11.256 | 41.231 | 70.406 | 1.00 | 18.53 |
| 40 | ATOM | 2970 | CD2 | TYR | A | 378 | 11.536 | 43.331 | 71.543 | 1.00 | 18.47 |
|    | ATOM | 2971 | CE1 | TYR | A | 378 | 12.444 | 41.436 | 69.716 | 1.00 | 15.98 |
|    | ATOM | 2972 | CE2 | TYR | A | 378 | 12.719 | 43.555 | 70.840 | 1.00 | 18.77 |
|    | ATOM | 2973 | CZ  | TYR | A | 378 | 13.161 | 42.609 | 69.920 | 1.00 | 16.37 |
|    | ATOM | 2974 | OH  | TYR | A | 378 | 14.309 | 42.811 | 69.212 | 1.00 | 32.30 |
| 45 | ATOM | 2975 | N   | SER | A | 379 | 11.879 | 40.317 | 73.977 | 1.00 | 23.03 |
|    | ATOM | 2976 | CA  | SER | A | 379 | 13.115 | 40.430 | 74.725 | 1.00 | 18.13 |
|    | ATOM | 2977 | C   | SER | A | 379 | 14.267 | 39.777 | 73.970 | 1.00 | 20.60 |
|    | ATOM | 2978 | O   | SER | A | 379 | 14.100 | 39.334 | 72.843 | 1.00 | 18.46 |
|    | ATOM | 2979 | CB  | SER | A | 379 | 12.976 | 39.740 | 76.067 | 1.00 | 23.56 |
| 50 | ATOM | 2980 | OG  | SER | A | 379 | 12.805 | 38.329 | 75.883 | 1.00 | 37.26 |
|    | ATOM | 2981 | N   | SER | A | 380 | 15.424 | 39.697 | 74.651 | 1.00 | 23.65 |
|    | ATOM | 2982 | CA  | SER | A | 380 | 16.701 | 39.084 | 74.222 | 1.00 | 26.09 |
|    | ATOM | 2983 | C   | SER | A | 380 | 16.669 | 37.571 | 74.457 | 1.00 | 28.37 |
|    | ATOM | 2984 | O   | SER | A | 380 | 17.480 | 36.785 | 73.975 | 1.00 | 30.81 |
| 55 | ATOM | 2985 | CB  | SER | A | 380 | 17.889 | 39.588 | 75.062 | 1.00 | 31.60 |
|    | ATOM | 2986 | OG  | SER | A | 380 | 18.036 | 41.000 | 75.033 | 1.00 | 42.48 |
|    | ATOM | 2987 | N   | VAL | A | 381 | 15.718 | 37.188 | 75.260 | 1.00 | 18.04 |
|    | ATOM | 2988 | CA  | VAL | A | 381 | 15.595 | 35.812 | 75.598 | 1.00 | 14.91 |
|    | ATOM | 2989 | C   | VAL | A | 381 | 15.708 | 34.897 | 74.419 | 1.00 | 20.31 |
| 60 | ATOM | 2990 | O   | VAL | A | 381 | 16.620 | 34.091 | 74.330 | 1.00 | 27.64 |
|    | ATOM | 2991 | CB  | VAL | A | 381 | 14.408 | 35.546 | 76.501 | 1.00 | 16.34 |
|    | ATOM | 2992 | CG1 | VAL | A | 381 | 14.284 | 34.062 | 76.734 | 1.00 | 17.26 |
|    | ATOM | 2993 | CG2 | VAL | A | 381 | 14.687 | 36.204 | 77.829 | 1.00 | 13.94 |
|    | ATOM | 2994 | N   | PRO | A | 382 | 14.797 | 35.005 | 73.489 | 1.00 | 16.53 |
|    | ATOM | 2995 | CA  | PRO | A | 382 | 14.886 | 34.139 | 72.324 | 1.00 | 17.21 |
|    | ATOM | 2996 | C   | PRO | A | 382 | 16.222 | 34.230 | 71.634 | 1.00 | 24.01 |
|    | ATOM | 2997 | O   | PRO | A | 382 | 16.709 | 33.192 | 71.207 | 1.00 | 27.79 |
|    | ATOM | 2998 | CB  | PRO | A | 382 | 13.777 | 34.514 | 71.351 | 1.00 | 17.20 |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
|    | ATOM | 2999 | CG  | PRO | A | 382 | 13.003 | 35.618 | 72.033 | 1.00 | 18.32 |
|    | ATOM | 3000 | CD  | PRO | A | 382 | 13.627 | 35.873 | 73.399 | 1.00 | 12.12 |
|    | ATOM | 3001 | N   | TYR | A | 383 | 16.809 | 35.447 | 71.542 | 1.00 | 19.33 |
| 5  | ATOM | 3002 | CA  | TYR | A | 383 | 18.112 | 35.648 | 70.902 | 1.00 | 19.70 |
|    | ATOM | 3003 | C   | TYR | A | 383 | 19.246 | 34.953 | 71.651 | 1.00 | 28.79 |
|    | ATOM | 3004 | O   | TYR | A | 383 | 19.980 | 34.117 | 71.104 | 1.00 | 31.38 |
|    | ATOM | 3005 | CB  | TYR | A | 383 | 18.468 | 37.135 | 70.894 | 1.00 | 21.02 |
|    | ATOM | 3006 | CG  | TYR | A | 383 | 17.593 | 37.968 | 70.011 | 1.00 | 23.86 |
| 10 | ATOM | 3007 | CD1 | TYR | A | 383 | 16.290 | 38.277 | 70.404 | 1.00 | 28.36 |
|    | ATOM | 3008 | CD2 | TYR | A | 383 | 18.067 | 38.450 | 68.784 | 1.00 | 20.93 |
|    | ATOM | 3009 | CE1 | TYR | A | 383 | 15.473 | 39.054 | 69.576 | 1.00 | 30.88 |
|    | ATOM | 3010 | CE2 | TYR | A | 383 | 17.272 | 39.244 | 67.957 | 1.00 | 18.71 |
|    | ATOM | 3011 | CZ  | TYR | A | 383 | 15.967 | 39.533 | 68.358 | 1.00 | 25.95 |
|    | ATOM | 3012 | OH  | TYR | A | 383 | 15.171 | 40.294 | 67.556 | 1.00 | 30.84 |
| 15 | ATOM | 3013 | N   | GLU | A | 384 | 19.389 | 35.333 | 72.921 | 1.00 | 20.17 |
|    | ATOM | 3014 | CA  | GLU | A | 384 | 20.419 | 34.857 | 73.803 | 1.00 | 17.57 |
|    | ATOM | 3015 | C   | GLU | A | 384 | 20.188 | 33.506 | 74.405 | 1.00 | 22.88 |
|    | ATOM | 3016 | O   | GLU | A | 384 | 21.151 | 32.775 | 74.669 | 1.00 | 25.65 |
| 20 | ATOM | 3017 | CB  | GLU | A | 384 | 20.833 | 35.973 | 74.773 | 1.00 | 20.44 |
|    | ATOM | 3018 | CG  | GLU | A | 384 | 21.263 | 37.202 | 73.944 | 1.00 | 15.21 |
|    | ATOM | 3019 | CD  | GLU | A | 384 | 22.539 | 36.937 | 73.184 | 1.00 | 26.58 |
|    | ATOM | 3020 | OE1 | GLU | A | 384 | 23.185 | 35.915 | 73.293 | 1.00 | 17.84 |
|    | ATOM | 3021 | OE2 | GLU | A | 384 | 22.887 | 37.915 | 72.400 | 1.00 | 21.88 |
|    | ATOM | 3022 | N   | LYS | A | 385 | 18.935 | 33.116 | 74.610 | 1.00 | 20.33 |
| 25 | ATOM | 3023 | CA  | LYS | A | 385 | 18.736 | 31.767 | 75.146 | 1.00 | 20.05 |
|    | ATOM | 3024 | C   | LYS | A | 385 | 18.865 | 30.716 | 74.028 | 1.00 | 27.19 |
|    | ATOM | 3025 | O   | LYS | A | 385 | 19.420 | 29.621 | 74.219 | 1.00 | 31.66 |
|    | ATOM | 3026 | CB  | LYS | A | 385 | 17.507 | 31.577 | 76.014 | 1.00 | 21.51 |
|    | ATOM | 3027 | CG  | LYS | A | 385 | 17.676 | 30.384 | 76.953 | 1.00 | 22.29 |
| 30 | ATOM | 3028 | CD  | LYS | A | 385 | 16.386 | 29.820 | 77.518 | 1.00 | 19.87 |
|    | ATOM | 3029 | CE  | LYS | A | 385 | 16.049 | 30.277 | 78.937 | 1.00 | 31.60 |
|    | ATOM | 3030 | NZ  | LYS | A | 385 | 14.783 | 29.694 | 79.441 | 1.00 | 30.38 |
|    | ATOM | 3031 | N   | GLY | A | 386 | 18.364 | 31.084 | 72.832 | 1.00 | 20.72 |
|    | ATOM | 3032 | CA  | GLY | A | 386 | 18.453 | 30.248 | 71.637 | 1.00 | 17.41 |
| 35 | ATOM | 3033 | C   | GLY | A | 386 | 19.924 | 30.106 | 71.298 | 1.00 | 20.81 |
|    | ATOM | 3034 | O   | GLY | A | 386 | 20.396 | 29.001 | 71.225 | 1.00 | 22.50 |
|    | ATOM | 3035 | N   | PHE | A | 387 | 20.683 | 31.228 | 71.163 | 1.00 | 20.30 |
|    | ATOM | 3036 | CA  | PHE | A | 387 | 22.137 | 31.158 | 70.900 | 1.00 | 19.92 |
|    | ATOM | 3037 | C   | PHE | A | 387 | 22.840 | 30.263 | 71.905 | 1.00 | 29.09 |
| 40 | ATOM | 3038 | O   | PHE | A | 387 | 23.685 | 29.478 | 71.530 | 1.00 | 32.80 |
|    | ATOM | 3039 | CB  | PHE | A | 387 | 22.852 | 32.519 | 70.955 | 1.00 | 20.07 |
|    | ATOM | 3040 | CG  | PHE | A | 387 | 24.344 | 32.358 | 70.872 | 1.00 | 19.41 |
|    | ATOM | 3041 | CD1 | PHE | A | 387 | 24.949 | 32.163 | 69.631 | 1.00 | 19.67 |
|    | ATOM | 3042 | CD2 | PHE | A | 387 | 25.157 | 32.373 | 72.007 | 1.00 | 25.27 |
| 45 | ATOM | 3043 | CE1 | PHE | A | 387 | 26.329 | 31.977 | 69.525 | 1.00 | 20.88 |
|    | ATOM | 3044 | CE2 | PHE | A | 387 | 26.542 | 32.202 | 71.916 | 1.00 | 28.83 |
|    | ATOM | 3045 | CZ  | PHE | A | 387 | 27.131 | 31.981 | 70.668 | 1.00 | 23.24 |
|    | ATOM | 3046 | N   | ALA | A | 388 | 22.495 | 30.381 | 73.203 | 1.00 | 25.48 |
|    | ATOM | 3047 | CA  | ALA | A | 388 | 23.133 | 29.556 | 74.242 | 1.00 | 23.14 |
| 50 | ATOM | 3048 | C   | ALA | A | 388 | 22.872 | 28.108 | 74.055 | 1.00 | 32.10 |
|    | ATOM | 3049 | O   | ALA | A | 388 | 23.757 | 27.282 | 74.258 | 1.00 | 37.82 |
|    | ATOM | 3050 | CB  | ALA | A | 388 | 22.717 | 29.932 | 75.633 | 1.00 | 23.02 |
|    | ATOM | 3051 | N   | LEU | A | 389 | 21.636 | 27.793 | 73.691 | 1.00 | 26.31 |
|    | ATOM | 3052 | CA  | LEU | A | 389 | 21.275 | 26.405 | 73.460 | 1.00 | 21.42 |
| 55 | ATOM | 3053 | C   | LEU | A | 389 | 22.189 | 25.906 | 72.372 | 1.00 | 27.91 |
|    | ATOM | 3054 | O   | LEU | A | 389 | 22.865 | 24.900 | 72.532 | 1.00 | 29.25 |
|    | ATOM | 3055 | CB  | LEU | A | 389 | 19.841 | 26.300 | 72.937 | 1.00 | 19.24 |
|    | ATOM | 3056 | CG  | LEU | A | 389 | 19.427 | 24.868 | 72.632 | 1.00 | 17.17 |
|    | ATOM | 3057 | CD1 | LEU | A | 389 | 19.717 | 24.017 | 73.844 | 1.00 | 14.63 |
| 60 | ATOM | 3058 | CD2 | LEU | A | 389 | 17.943 | 24.808 | 72.328 | 1.00 | 10.16 |
|    | ATOM | 3059 | N   | LEU | A | 390 | 22.217 | 26.659 | 71.262 | 1.00 | 24.49 |
|    | ATOM | 3060 | CA  | LEU | A | 390 | 23.050 | 26.340 | 70.107 | 1.00 | 25.05 |
|    | ATOM | 3061 | C   | LEU | A | 390 | 24.531 | 26.256 | 70.383 | 1.00 | 32.31 |
|    | ATOM | 3062 | O   | LEU | A | 390 | 25.183 | 25.301 | 69.932 | 1.00 | 33.60 |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
|    | ATOM | 3063 | CB  | LEU | A | 390 | 22.765 | 27.152 | 68.844 | 1.00 | 23.33 |
|    | ATOM | 3064 | CG  | LEU | A | 390 | 21.307 | 27.026 | 68.442 | 1.00 | 23.38 |
|    | ATOM | 3065 | CD1 | LEU | A | 390 | 20.986 | 28.025 | 67.334 | 1.00 | 20.84 |
| 5  | ATOM | 3066 | CD2 | LEU | A | 390 | 20.988 | 25.591 | 68.017 | 1.00 | 18.86 |
|    | ATOM | 3067 | N   | PHE | A | 391 | 25.058 | 27.231 | 71.127 | 1.00 | 28.52 |
|    | ATOM | 3068 | CA  | PHE | A | 391 | 26.480 | 27.236 | 71.494 | 1.00 | 27.82 |
|    | ATOM | 3069 | C   | PHE | A | 391 | 26.813 | 25.992 | 72.312 | 1.00 | 28.67 |
|    | ATOM | 3070 | O   | PHE | A | 391 | 27.839 | 25.331 | 72.148 | 1.00 | 26.96 |
| 10 | ATOM | 3071 | CB  | PHE | A | 391 | 26.834 | 28.455 | 72.341 | 1.00 | 28.60 |
|    | ATOM | 3072 | CG  | PHE | A | 391 | 28.296 | 28.786 | 72.283 | 1.00 | 30.53 |
|    | ATOM | 3073 | CD1 | PHE | A | 391 | 28.967 | 28.816 | 71.064 | 1.00 | 35.08 |
|    | ATOM | 3074 | CD2 | PHE | A | 391 | 29.020 | 29.063 | 73.440 | 1.00 | 36.52 |
|    | ATOM | 3075 | CE1 | PHE | A | 391 | 30.320 | 29.142 | 70.983 | 1.00 | 37.61 |
|    | ATOM | 3076 | CE2 | PHE | A | 391 | 30.378 | 29.383 | 73.382 | 1.00 | 40.61 |
| 15 | ATOM | 3077 | CZ  | PHE | A | 391 | 31.026 | 29.432 | 72.148 | 1.00 | 37.64 |
|    | ATOM | 3078 | N   | TYR | A | 392 | 25.913 | 25.699 | 73.225 | 1.00 | 24.90 |
|    | ATOM | 3079 | CA  | TYR | A | 392 | 26.044 | 24.550 | 74.065 | 1.00 | 24.66 |
|    | ATOM | 3080 | C   | TYR | A | 392 | 26.106 | 23.298 | 73.186 | 1.00 | 34.30 |
| 20 | ATOM | 3081 | O   | TYR | A | 392 | 27.058 | 22.558 | 73.268 | 1.00 | 37.51 |
|    | ATOM | 3082 | CB  | TYR | A | 392 | 24.821 | 24.501 | 74.967 | 1.00 | 26.39 |
|    | ATOM | 3083 | CG  | TYR | A | 392 | 24.631 | 23.181 | 75.678 | 1.00 | 31.99 |
|    | ATOM | 3084 | CD1 | TYR | A | 392 | 25.546 | 22.715 | 76.625 | 1.00 | 35.17 |
|    | ATOM | 3085 | CD2 | TYR | A | 392 | 23.501 | 22.397 | 75.432 | 1.00 | 32.49 |
| 25 | ATOM | 3086 | CE1 | TYR | A | 392 | 25.341 | 21.512 | 77.306 | 1.00 | 39.01 |
|    | ATOM | 3087 | CE2 | TYR | A | 392 | 23.281 | 21.184 | 76.094 | 1.00 | 31.50 |
|    | ATOM | 3088 | CZ  | TYR | A | 392 | 24.206 | 20.743 | 77.035 | 1.00 | 34.08 |
|    | ATOM | 3089 | OH  | TYR | A | 392 | 23.986 | 19.564 | 77.683 | 1.00 | 36.46 |
|    | ATOM | 3090 | N   | LEU | A | 393 | 25.101 | 23.067 | 72.310 | 1.00 | 31.02 |
| 30 | ATOM | 3091 | CA  | LEU | A | 393 | 25.043 | 21.889 | 71.410 | 1.00 | 29.65 |
|    | ATOM | 3092 | C   | LEU | A | 393 | 26.274 | 21.616 | 70.507 | 1.00 | 32.03 |
|    | ATOM | 3093 | O   | LEU | A | 393 | 26.664 | 20.468 | 70.267 | 1.00 | 27.90 |
|    | ATOM | 3094 | CB  | LEU | A | 393 | 23.758 | 21.905 | 70.552 | 1.00 | 28.85 |
|    | ATOM | 3095 | CG  | LEU | A | 393 | 22.489 | 21.688 | 71.375 | 1.00 | 30.33 |
| 35 | ATOM | 3096 | CD1 | LEU | A | 393 | 21.256 | 22.047 | 70.559 | 1.00 | 27.38 |
|    | ATOM | 3097 | CD2 | LEU | A | 393 | 22.400 | 20.246 | 71.865 | 1.00 | 29.76 |
|    | ATOM | 3098 | N   | GLU | A | 394 | 26.841 | 22.701 | 69.980 | 1.00 | 30.84 |
|    | ATOM | 3099 | CA  | GLU | A | 394 | 28.000 | 22.727 | 69.118 | 1.00 | 30.05 |
|    | ATOM | 3100 | C   | GLU | A | 394 | 29.210 | 22.214 | 69.868 | 1.00 | 39.16 |
| 40 | ATOM | 3101 | O   | GLU | A | 394 | 30.089 | 21.595 | 69.299 | 1.00 | 42.14 |
|    | ATOM | 3102 | CB  | GLU | A | 394 | 28.300 | 24.204 | 68.756 | 1.00 | 31.03 |
|    | ATOM | 3103 | CG  | GLU | A | 394 | 29.776 | 24.406 | 68.376 | 1.00 | 37.11 |
|    | ATOM | 3104 | CD  | GLU | A | 394 | 30.182 | 25.830 | 68.208 | 1.00 | 45.20 |
|    | ATOM | 3105 | OE1 | GLU | A | 394 | 29.614 | 26.609 | 67.471 | 1.00 | 56.77 |
| 45 | ATOM | 3106 | OE2 | GLU | A | 394 | 31.229 | 26.133 | 68.927 | 1.00 | 39.77 |
|    | ATOM | 3107 | N   | GLN | A | 395 | 29.256 | 22.534 | 71.160 | 1.00 | 34.20 |
|    | ATOM | 3108 | CA  | GLN | A | 395 | 30.342 | 22.139 | 72.029 | 1.00 | 32.86 |
|    | ATOM | 3109 | C   | GLN | A | 395 | 30.143 | 20.690 | 72.435 | 1.00 | 38.65 |
|    | ATOM | 3110 | O   | GLN | A | 395 | 31.066 | 19.899 | 72.507 | 1.00 | 38.67 |
| 50 | ATOM | 3111 | CB  | GLN | A | 395 | 30.474 | 23.051 | 73.287 | 1.00 | 33.17 |
|    | ATOM | 3112 | CG  | GLN | A | 395 | 30.831 | 24.540 | 72.996 | 1.00 | 13.79 |
|    | ATOM | 3113 | CD  | GLN | A | 395 | 31.176 | 25.354 | 74.247 | 1.00 | 37.45 |
|    | ATOM | 3114 | OE1 | GLN | A | 395 | 30.909 | 24.959 | 75.407 | 1.00 | 26.89 |
|    | ATOM | 3115 | NE2 | GLN | A | 395 | 31.758 | 26.523 | 74.010 | 1.00 | 31.99 |
| 55 | ATOM | 3116 | N   | LEU | A | 396 | 28.903 | 20.352 | 72.682 | 1.00 | 38.68 |
|    | ATOM | 3117 | CA  | LEU | A | 396 | 28.514 | 19.015 | 73.083 | 1.00 | 38.49 |
|    | ATOM | 3118 | C   | LEU | A | 396 | 28.633 | 18.017 | 71.924 | 1.00 | 39.28 |
|    | ATOM | 3119 | O   | LEU | A | 396 | 29.012 | 16.871 | 72.100 | 1.00 | 42.17 |
|    | ATOM | 3120 | CB  | LEU | A | 396 | 27.055 | 19.072 | 73.628 | 1.00 | 37.93 |
| 60 | ATOM | 3121 | CG  | LEU | A | 396 | 26.389 | 17.732 | 73.946 | 1.00 | 42.72 |
|    | ATOM | 3122 | CD1 | LEU | A | 396 | 26.436 | 17.489 | 75.445 | 1.00 | 45.42 |
|    | ATOM | 3123 | CD2 | LEU | A | 396 | 24.917 | 17.709 | 73.527 | 1.00 | 43.81 |
|    | ATOM | 3124 | N   | LEU | A | 397 | 28.303 | 18.456 | 70.730 | 1.00 | 28.48 |
|    | ATOM | 3125 | CA  | LEU | A | 397 | 28.337 | 17.595 | 69.589 | 1.00 | 25.49 |
|    | ATOM | 3126 | C   | LEU | A | 397 | 29.620 | 17.609 | 68.771 | 1.00 | 36.86 |



|    |      |      |     |     |   |     |        |        |        |      |        |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
| 5  | ATOM | 3127 | O   | LEU | A | 397 | 29.596 | 17.220 | 67.599 | 1.00 | 39.85  |
|    | ATOM | 3128 | CB  | LEU | A | 397 | 27.156 | 17.924 | 68.686 | 1.00 | 23.73  |
|    | ATOM | 3129 | CG  | LEU | A | 397 | 25.843 | 17.773 | 69.401 | 1.00 | 25.82  |
|    | ATOM | 3130 | CD1 | LEU | A | 397 | 24.740 | 18.559 | 68.669 | 1.00 | 22.99  |
|    | ATOM | 3131 | CD2 | LEU | A | 397 | 25.525 | 16.272 | 69.452 | 1.00 | 27.30  |
| 10 | ATOM | 3132 | N   | GLY | A | 398 | 30.731 | 18.069 | 69.342 | 1.00 | 33.98  |
|    | ATOM | 3133 | CA  | GLY | A | 398 | 31.993 | 18.038 | 68.617 | 1.00 | 34.14  |
|    | ATOM | 3134 | C   | GLY | A | 398 | 32.547 | 19.260 | 67.889 | 1.00 | 38.92  |
|    | ATOM | 3135 | O   | GLY | A | 398 | 33.502 | 19.097 | 67.115 | 1.00 | 39.98  |
|    | ATOM | 3136 | N   | GLY | A | 399 | 32.001 | 20.457 | 68.105 | 1.00 | 33.01  |
| 15 | ATOM | 3137 | CA  | GLY | A | 399 | 32.543 | 21.650 | 67.440 | 1.00 | 30.35  |
|    | ATOM | 3138 | C   | GLY | A | 399 | 31.713 | 22.336 | 66.365 | 1.00 | 31.72  |
|    | ATOM | 3139 | O   | GLY | A | 399 | 30.800 | 21.823 | 65.762 | 1.00 | 34.57  |
|    | ATOM | 3140 | N   | PRO | A | 400 | 32.076 | 23.550 | 66.124 | 1.00 | 33.01  |
|    | ATOM | 3141 | CA  | PRO | A | 400 | 31.429 | 24.406 | 65.151 | 1.00 | 35.02  |
| 20 | ATOM | 3142 | C   | PRO | A | 400 | 31.379 | 23.794 | 63.750 | 1.00 | 43.93  |
|    | ATOM | 3143 | O   | PRO | A | 400 | 30.360 | 23.838 | 63.045 | 1.00 | 40.14  |
|    | ATOM | 3144 | CB  | PRO | A | 400 | 32.293 | 25.672 | 65.111 | 1.00 | 35.73  |
|    | ATOM | 3145 | CG  | PRO | A | 400 | 33.539 | 25.411 | 65.948 | 1.00 | 38.03  |
|    | ATOM | 3146 | CD  | PRO | A | 400 | 33.423 | 24.010 | 66.517 | 1.00 | 33.92  |
| 25 | ATOM | 3147 | N   | GLU | A | 401 | 32.512 | 23.237 | 63.345 | 1.00 | 43.85  |
|    | ATOM | 3148 | CA  | GLU | A | 401 | 32.597 | 22.620 | 62.042 | 1.00 | 42.92  |
|    | ATOM | 3149 | C   | GLU | A | 401 | 31.491 | 21.587 | 61.878 | 1.00 | 37.92  |
|    | ATOM | 3150 | O   | GLU | A | 401 | 30.810 | 21.588 | 60.866 | 1.00 | 33.79  |
|    | ATOM | 3151 | CB  | GLU | A | 401 | 33.996 | 22.034 | 61.789 | 1.00 | 45.93  |
| 30 | ATOM | 3152 | CG  | GLU | A | 401 | 34.578 | 22.372 | 60.398 | 1.00 | 69.62  |
|    | ATOM | 3153 | CD  | GLU | A | 401 | 35.603 | 21.373 | 59.911 | 1.00 | 100.00 |
|    | ATOM | 3154 | OE1 | GLU | A | 401 | 36.702 | 21.236 | 60.427 | 1.00 | 100.00 |
|    | ATOM | 3155 | OE2 | GLU | A | 401 | 35.195 | 20.689 | 58.865 | 1.00 | 93.16  |
|    | ATOM | 3156 | N   | ILE | A | 402 | 31.317 | 20.720 | 62.902 | 1.00 | 34.58  |
| 35 | ATOM | 3157 | CA  | ILE | A | 402 | 30.281 | 19.681 | 62.922 | 1.00 | 33.20  |
|    | ATOM | 3158 | C   | ILE | A | 402 | 28.898 | 20.291 | 62.938 | 1.00 | 39.09  |
|    | ATOM | 3159 | O   | ILE | A | 402 | 28.065 | 19.896 | 62.133 | 1.00 | 41.43  |
|    | ATOM | 3160 | CB  | ILE | A | 402 | 30.391 | 18.673 | 64.078 | 1.00 | 33.82  |
|    | ATOM | 3161 | CG1 | ILE | A | 402 | 31.490 | 17.661 | 63.811 | 1.00 | 34.70  |
| 40 | ATOM | 3162 | CG2 | ILE | A | 402 | 29.080 | 17.900 | 64.287 | 1.00 | 23.32  |
|    | ATOM | 3163 | CD1 | ILE | A | 402 | 31.878 | 16.896 | 65.080 | 1.00 | 49.20  |
|    | ATOM | 3164 | N   | PHE | A | 403 | 28.668 | 21.246 | 63.868 | 1.00 | 32.73  |
|    | ATOM | 3165 | CA  | PHE | A | 403 | 27.390 | 21.952 | 64.044 | 1.00 | 29.52  |
|    | ATOM | 3166 | C   | PHE | A | 403 | 27.032 | 22.816 | 62.836 | 1.00 | 33.94  |
| 45 | ATOM | 3167 | O   | PHE | A | 403 | 25.866 | 23.022 | 62.469 | 1.00 | 34.15  |
|    | ATOM | 3168 | CB  | PHE | A | 403 | 27.319 | 22.719 | 65.381 | 1.00 | 29.03  |
|    | ATOM | 3169 | CG  | PHE | A | 403 | 25.917 | 22.783 | 65.929 | 1.00 | 28.54  |
|    | ATOM | 3170 | CD1 | PHE | A | 403 | 25.323 | 21.643 | 66.484 | 1.00 | 29.91  |
|    | ATOM | 3171 | CD2 | PHE | A | 403 | 25.176 | 23.964 | 65.873 | 1.00 | 27.62  |
| 50 | ATOM | 3172 | CE1 | PHE | A | 403 | 24.021 | 21.667 | 66.990 | 1.00 | 27.38  |
|    | ATOM | 3173 | CE2 | PHE | A | 403 | 23.881 | 24.017 | 66.393 | 1.00 | 28.82  |
|    | ATOM | 3174 | CZ  | PHE | A | 403 | 23.304 | 22.863 | 66.932 | 1.00 | 25.72  |
|    | ATOM | 3175 | N   | LEU | A | 404 | 28.040 | 23.327 | 62.165 | 1.00 | 31.31  |
|    | ATOM | 3176 | CA  | LEU | A | 404 | 27.687 | 24.080 | 60.983 | 1.00 | 32.95  |
| 55 | ATOM | 3177 | C   | LEU | A | 404 | 27.068 | 23.099 | 59.952 | 1.00 | 32.89  |
|    | ATOM | 3178 | O   | LEU | A | 404 | 26.050 | 23.361 | 59.315 | 1.00 | 37.36  |
|    | ATOM | 3179 | CB  | LEU | A | 404 | 28.798 | 25.045 | 60.464 | 1.00 | 33.15  |
|    | ATOM | 3180 | CG  | LEU | A | 404 | 29.029 | 26.208 | 61.444 | 1.00 | 36.96  |
|    | ATOM | 3181 | CD1 | LEU | A | 404 | 30.454 | 26.717 | 61.353 | 1.00 | 37.13  |
| 60 | ATOM | 3182 | CD2 | LEU | A | 404 | 28.083 | 27.362 | 61.163 | 1.00 | 39.27  |
|    | ATOM | 3183 | N   | GLY | A | 405 | 27.670 | 21.921 | 59.826 | 1.00 | 22.02  |
|    | ATOM | 3184 | CA  | GLY | A | 405 | 27.167 | 20.908 | 58.928 | 1.00 | 22.77  |
|    | ATOM | 3185 | C   | GLY | A | 405 | 25.698 | 20.676 | 59.206 | 1.00 | 31.85  |
|    | ATOM | 3186 | O   | GLY | A | 405 | 24.885 | 20.438 | 58.297 | 1.00 | 33.01  |
|    | ATOM | 3187 | N   | PHE | A | 406 | 25.364 | 20.747 | 60.493 | 1.00 | 26.28  |
|    | ATOM | 3188 | CA  | PHE | A | 406 | 23.992 | 20.565 | 60.863 | 1.00 | 25.27  |
|    | ATOM | 3189 | C   | PHE | A | 406 | 23.188 | 21.757 | 60.365 | 1.00 | 34.80  |
|    | ATOM | 3190 | O   | PHE | A | 406 | 22.195 | 21.629 | 59.638 | 1.00 | 36.22  |



|    |      |      |     |           |        |        |        |      |        |
|----|------|------|-----|-----------|--------|--------|--------|------|--------|
|    | ATOM | 3191 | CB  | PHE A 406 | 23.798 | 20.268 | 62.351 | 1.00 | 24.52  |
|    | ATOM | 3192 | CG  | PHE A 406 | 22.388 | 20.525 | 62.798 | 1.00 | 24.82  |
|    | ATOM | 3193 | CD1 | PHE A 406 | 21.328 | 19.734 | 62.353 | 1.00 | 28.50  |
|    | ATOM | 3194 | CD2 | PHE A 406 | 22.107 | 21.579 | 63.669 | 1.00 | 30.12  |
| 5  | ATOM | 3195 | CE1 | PHE A 406 | 20.025 | 19.977 | 62.793 | 1.00 | 31.40  |
|    | ATOM | 3196 | CE2 | PHE A 406 | 20.810 | 21.862 | 64.105 | 1.00 | 32.57  |
|    | ATOM | 3197 | CZ  | PHE A 406 | 19.771 | 21.037 | 63.669 | 1.00 | 31.88  |
|    | ATOM | 3198 | N   | LEU A 407 | 23.661 | 22.934 | 60.708 | 1.00 | 32.11  |
| 10 | ATOM | 3199 | CA  | LEU A 407 | 22.972 | 24.132 | 60.269 | 1.00 | 33.11  |
|    | ATOM | 3200 | C   | LEU A 407 | 22.706 | 24.204 | 58.767 | 1.00 | 34.74  |
|    | ATOM | 3201 | O   | LEU A 407 | 21.635 | 24.615 | 58.341 | 1.00 | 35.21  |
|    | ATOM | 3202 | CB  | LEU A 407 | 23.589 | 25.420 | 60.840 | 1.00 | 35.36  |
|    | ATOM | 3203 | CG  | LEU A 407 | 22.597 | 26.577 | 60.855 | 1.00 | 41.79  |
|    | ATOM | 3204 | CD1 | LEU A 407 | 23.048 | 27.626 | 61.833 | 1.00 | 40.45  |
| 15 | ATOM | 3205 | CD2 | LEU A 407 | 22.513 | 27.197 | 59.461 | 1.00 | 49.57  |
|    | ATOM | 3206 | N   | LYS A 408 | 23.667 | 23.804 | 57.948 | 1.00 | 34.92  |
|    | ATOM | 3207 | CA  | LYS A 408 | 23.476 | 23.826 | 56.490 | 1.00 | 36.29  |
|    | ATOM | 3208 | C   | LYS A 408 | 22.378 | 22.876 | 56.037 | 1.00 | 38.15  |
| 20 | ATOM | 3209 | O   | LYS A 408 | 21.568 | 23.191 | 55.160 | 1.00 | 35.09  |
|    | ATOM | 3210 | CB  | LYS A 408 | 24.747 | 23.517 | 55.707 | 1.00 | 40.54  |
|    | ATOM | 3211 | CG  | LYS A 408 | 24.633 | 23.873 | 54.214 | 1.00 | 43.41  |
|    | ATOM | 3212 | CD  | LYS A 408 | 25.950 | 23.796 | 53.422 | 1.00 | 49.26  |
|    | ATOM | 3213 | CE  | LYS A 408 | 26.808 | 25.059 | 53.459 | 1.00 | 61.45  |
|    | ATOM | 3214 | NZ  | LYS A 408 | 28.014 | 24.994 | 52.606 | 1.00 | 73.78  |
| 25 | ATOM | 3215 | N   | ALA A 409 | 22.352 | 21.690 | 56.655 | 1.00 | 35.34  |
|    | ATOM | 3216 | CA  | ALA A 409 | 21.333 | 20.698 | 56.298 | 1.00 | 36.14  |
|    | ATOM | 3217 | C   | ALA A 409 | 19.927 | 21.041 | 56.814 | 1.00 | 38.45  |
|    | ATOM | 3218 | O   | ALA A 409 | 18.913 | 20.821 | 56.134 | 1.00 | 37.39  |
| 30 | ATOM | 3219 | CB  | ALA A 409 | 21.762 | 19.273 | 56.626 | 1.00 | 36.66  |
|    | ATOM | 3220 | N   | TYR A 410 | 19.902 | 21.597 | 58.030 | 1.00 | 33.14  |
|    | ATOM | 3221 | CA  | TYR A 410 | 18.693 | 22.059 | 58.682 | 1.00 | 29.65  |
|    | ATOM | 3222 | C   | TYR A 410 | 18.028 | 23.051 | 57.730 | 1.00 | 35.55  |
|    | ATOM | 3223 | O   | TYR A 410 | 16.855 | 22.976 | 57.399 | 1.00 | 37.26  |
| 35 | ATOM | 3224 | CB  | TYR A 410 | 19.117 | 22.762 | 59.970 | 1.00 | 24.67  |
|    | ATOM | 3225 | CG  | TYR A 410 | 18.069 | 23.643 | 60.541 | 1.00 | 26.95  |
|    | ATOM | 3226 | CD1 | TYR A 410 | 16.861 | 23.112 | 60.990 | 1.00 | 28.10  |
|    | ATOM | 3227 | CD2 | TYR A 410 | 18.288 | 25.015 | 60.663 | 1.00 | 29.66  |
|    | ATOM | 3228 | CE1 | TYR A 410 | 15.883 | 23.924 | 61.571 | 1.00 | 26.98  |
| 40 | ATOM | 3229 | CE2 | TYR A 410 | 17.316 | 25.839 | 61.230 | 1.00 | 31.84  |
|    | ATOM | 3230 | CZ  | TYR A 410 | 16.112 | 25.294 | 61.685 | 1.00 | 37.49  |
|    | ATOM | 3231 | OH  | TYR A 410 | 15.156 | 26.110 | 62.241 | 1.00 | 33.48  |
|    | ATOM | 3232 | N   | VAL A 411 | 18.848 | 23.961 | 57.262 | 1.00 | 28.75  |
|    | ATOM | 3233 | CA  | VAL A 411 | 18.457 | 24.984 | 56.341 | 1.00 | 29.23  |
| 45 | ATOM | 3234 | C   | VAL A 411 | 18.013 | 24.469 | 54.992 | 1.00 | 34.00  |
|    | ATOM | 3235 | O   | VAL A 411 | 17.060 | 24.982 | 54.401 | 1.00 | 30.00  |
|    | ATOM | 3236 | CB  | VAL A 411 | 19.617 | 25.922 | 56.139 | 1.00 | 32.22  |
|    | ATOM | 3237 | CG1 | VAL A 411 | 19.331 | 26.821 | 54.950 | 1.00 | 29.86  |
|    | ATOM | 3238 | CG2 | VAL A 411 | 19.850 | 26.708 | 57.431 | 1.00 | 31.69  |
| 50 | ATOM | 3239 | N   | GLU A 412 | 18.730 | 23.479 | 54.488 | 1.00 | 33.14  |
|    | ATOM | 3240 | CA  | GLU A 412 | 18.402 | 22.900 | 53.217 | 1.00 | 31.91  |
|    | ATOM | 3241 | C   | GLU A 412 | 17.068 | 22.163 | 53.355 | 1.00 | 30.32  |
|    | ATOM | 3242 | O   | GLU A 412 | 16.182 | 22.225 | 52.531 | 1.00 | 31.89  |
|    | ATOM | 3243 | CB  | GLU A 412 | 19.502 | 21.883 | 52.932 | 1.00 | 36.48  |
| 55 | ATOM | 3244 | CG  | GLU A 412 | 20.443 | 22.174 | 51.737 | 1.00 | 67.01  |
|    | ATOM | 3245 | CD  | GLU A 412 | 21.872 | 21.699 | 51.962 | 1.00 | 100.00 |
|    | ATOM | 3246 | OE1 | GLU A 412 | 22.193 | 20.782 | 52.716 | 1.00 | 100.00 |
|    | ATOM | 3247 | OE2 | GLU A 412 | 22.750 | 22.396 | 51.277 | 1.00 | 94.73  |
|    | ATOM | 3248 | N   | LYS A 413 | 16.922 | 21.444 | 54.444 | 1.00 | 22.18  |
| 60 | ATOM | 3249 | CA  | LYS A 413 | 15.729 | 20.692 | 54.714 | 1.00 | 17.91  |
|    | ATOM | 3250 | C   | LYS A 413 | 14.463 | 21.486 | 54.855 | 1.00 | 23.75  |
|    | ATOM | 3251 | O   | LYS A 413 | 13.417 | 20.978 | 54.503 | 1.00 | 25.92  |
|    | ATOM | 3252 | CB  | LYS A 413 | 15.890 | 19.911 | 55.988 | 1.00 | 15.65  |
|    | ATOM | 3253 | CG  | LYS A 413 | 14.554 | 19.422 | 56.503 | 1.00 | 38.69  |
|    | ATOM | 3254 | CD  | LYS A 413 | 14.150 | 18.089 | 55.903 | 1.00 | 58.11  |



|    |      |      |     |     |   |     |        |        |        |      |        |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
|    | ATOM | 3255 | CE  | LYS | A | 413 | 13.634 | 17.099 | 56.937 | 1.00 | 64.98  |
|    | ATOM | 3256 | NZ  | LYS | A | 413 | 13.457 | 15.751 | 56.381 | 1.00 | 73.89  |
|    | ATOM | 3257 | N   | PHE | A | 414 | 14.530 | 22.688 | 55.424 | 1.00 | 25.40  |
| 5  | ATOM | 3258 | CA  | PHE | A | 414 | 13.316 | 23.479 | 55.640 | 1.00 | 27.80  |
|    | ATOM | 3259 | C   | PHE | A | 414 | 13.151 | 24.748 | 54.821 | 1.00 | 35.82  |
|    | ATOM | 3260 | O   | PHE | A | 414 | 12.276 | 25.557 | 55.122 | 1.00 | 35.17  |
|    | ATOM | 3261 | CB  | PHE | A | 414 | 13.063 | 23.791 | 57.118 | 1.00 | 30.46  |
|    | ATOM | 3262 | CG  | PHE | A | 414 | 12.936 | 22.553 | 57.964 | 1.00 | 33.88  |
| 10 | ATOM | 3263 | CD1 | PHE | A | 414 | 11.746 | 21.826 | 57.996 | 1.00 | 35.94  |
|    | ATOM | 3264 | CD2 | PHE | A | 414 | 14.005 | 22.110 | 58.742 | 1.00 | 37.75  |
|    | ATOM | 3265 | CE1 | PHE | A | 414 | 11.629 | 20.664 | 58.761 | 1.00 | 37.77  |
|    | ATOM | 3266 | CE2 | PHE | A | 414 | 13.888 | 20.962 | 59.526 | 1.00 | 42.23  |
|    | ATOM | 3267 | CZ  | PHE | A | 414 | 12.698 | 20.231 | 59.542 | 1.00 | 39.10  |
| 15 | ATOM | 3268 | N   | SER | A | 415 | 13.970 | 24.933 | 53.795 | 1.00 | 36.12  |
|    | ATOM | 3269 | CA  | SER | A | 415 | 13.858 | 26.115 | 52.945 | 1.00 | 36.36  |
|    | ATOM | 3270 | C   | SER | A | 415 | 12.412 | 26.295 | 52.510 | 1.00 | 38.99  |
|    | ATOM | 3271 | O   | SER | A | 415 | 11.730 | 25.315 | 52.243 | 1.00 | 41.04  |
|    | ATOM | 3272 | CB  | SER | A | 415 | 14.773 | 26.008 | 51.736 | 1.00 | 37.43  |
| 20 | ATOM | 3273 | OG  | SER | A | 415 | 16.036 | 26.566 | 52.046 | 1.00 | 46.73  |
|    | ATOM | 3274 | N   | TYR | A | 416 | 11.928 | 27.537 | 52.475 | 1.00 | 33.40  |
|    | ATOM | 3275 | CA  | TYR | A | 416 | 10.541 | 27.832 | 52.072 | 1.00 | 30.88  |
|    | ATOM | 3276 | C   | TYR | A | 416 | 9.453  | 27.183 | 52.947 | 1.00 | 33.62  |
|    | ATOM | 3277 | O   | TYR | A | 416 | 8.295  | 27.095 | 52.546 | 1.00 | 33.44  |
| 25 | ATOM | 3278 | CB  | TYR | A | 416 | 10.292 | 27.479 | 50.584 | 1.00 | 28.42  |
|    | ATOM | 3279 | CG  | TYR | A | 416 | 11.496 | 27.782 | 49.723 | 1.00 | 24.76  |
|    | ATOM | 3280 | CD1 | TYR | A | 416 | 11.791 | 29.087 | 49.338 | 1.00 | 26.55  |
|    | ATOM | 3281 | CD2 | TYR | A | 416 | 12.375 | 26.778 | 49.335 | 1.00 | 21.68  |
|    | ATOM | 3282 | CE1 | TYR | A | 416 | 12.914 | 29.384 | 48.570 | 1.00 | 25.16  |
| 30 | ATOM | 3283 | CE2 | TYR | A | 416 | 13.504 | 27.052 | 48.572 | 1.00 | 20.15  |
|    | ATOM | 3284 | CZ  | TYR | A | 416 | 13.780 | 28.360 | 48.189 | 1.00 | 30.62  |
|    | ATOM | 3285 | OH  | TYR | A | 416 | 14.892 | 28.616 | 47.399 | 1.00 | 35.15  |
|    | ATOM | 3286 | N   | LYS | A | 417 | 9.823  | 26.713 | 54.122 | 1.00 | 27.67  |
|    | ATOM | 3287 | CA  | LYS | A | 417 | 8.889  | 26.065 | 55.008 | 1.00 | 28.02  |
| 35 | ATOM | 3288 | C   | LYS | A | 417 | 8.733  | 26.830 | 56.317 | 1.00 | 31.36  |
|    | ATOM | 3289 | O   | LYS | A | 417 | 9.547  | 27.671 | 56.682 | 1.00 | 33.15  |
|    | ATOM | 3290 | CB  | LYS | A | 417 | 9.335  | 24.615 | 55.252 | 1.00 | 33.86  |
|    | ATOM | 3291 | CG  | LYS | A | 417 | 8.449  | 23.792 | 56.201 | 1.00 | 86.28  |
|    | ATOM | 3292 | CD  | LYS | A | 417 | 8.742  | 22.275 | 56.232 | 1.00 | 100.00 |
| 40 | ATOM | 3293 | CE  | LYS | A | 417 | 7.924  | 21.471 | 57.265 | 1.00 | 72.28  |
|    | ATOM | 3294 | NZ  | LYS | A | 417 | 8.280  | 20.033 | 57.323 | 1.00 | 41.88  |
|    | ATOM | 3295 | N   | SER | A | 418 | 7.668  | 26.557 | 57.033 | 1.00 | 28.88  |
|    | ATOM | 3296 | CA  | SER | A | 418 | 7.455  | 27.195 | 58.335 | 1.00 | 30.04  |
|    | ATOM | 3297 | C   | SER | A | 418 | 7.425  | 26.064 | 59.332 | 1.00 | 34.09  |
| 45 | ATOM | 3298 | O   | SER | A | 418 | 6.614  | 25.145 | 59.193 | 1.00 | 31.54  |
|    | ATOM | 3299 | CB  | SER | A | 418 | 6.261  | 28.126 | 58.410 | 1.00 | 31.46  |
|    | ATOM | 3300 | OG  | SER | A | 418 | 6.417  | 29.106 | 57.399 | 1.00 | 35.01  |
|    | ATOM | 3301 | N   | ILE | A | 419 | 8.356  | 26.077 | 60.281 | 1.00 | 28.50  |
|    | ATOM | 3302 | CA  | ILE | A | 419 | 8.446  | 24.971 | 61.205 | 1.00 | 23.86  |
| 50 | ATOM | 3303 | C   | ILE | A | 419 | 8.272  | 25.342 | 62.641 | 1.00 | 25.06  |
|    | ATOM | 3304 | O   | ILE | A | 419 | 8.122  | 26.500 | 63.002 | 1.00 | 21.64  |
|    | ATOM | 3305 | CB  | ILE | A | 419 | 9.803  | 24.314 | 61.026 | 1.00 | 25.02  |
|    | ATOM | 3306 | CG1 | ILE | A | 419 | 10.863 | 25.325 | 61.399 | 1.00 | 23.63  |
|    | ATOM | 3307 | CG2 | ILE | A | 419 | 10.051 | 23.937 | 59.565 | 1.00 | 23.22  |
| 55 | ATOM | 3308 | CD1 | ILE | A | 419 | 12.236 | 24.688 | 61.253 | 1.00 | 23.48  |
|    | ATOM | 3309 | N   | THR | A | 420 | 8.321  | 24.302 | 63.455 | 1.00 | 24.71  |
|    | ATOM | 3310 | CA  | THR | A | 420 | 8.201  | 24.417 | 64.895 | 1.00 | 24.36  |
|    | ATOM | 3311 | C   | THR | A | 420 | 9.416  | 23.795 | 65.538 | 1.00 | 28.90  |
|    | ATOM | 3312 | O   | THR | A | 420 | 10.190 | 23.112 | 64.863 | 1.00 | 23.38  |
| 60 | ATOM | 3313 | CB  | THR | A | 420 | 6.979  | 23.691 | 65.448 | 1.00 | 24.92  |
|    | ATOM | 3314 | OG1 | THR | A | 420 | 7.190  | 22.313 | 65.291 | 1.00 | 26.43  |
|    | ATOM | 3315 | CG2 | THR | A | 420 | 5.728  | 24.082 | 64.694 | 1.00 | 31.57  |
|    | ATOM | 3316 | N   | THR | A | 421 | 9.542  | 24.051 | 66.855 | 1.00 | 29.30  |
|    | ATOM | 3317 | CA  | THR | A | 421 | 10.610 | 23.549 | 67.709 | 1.00 | 27.78  |
|    | ATOM | 3318 | C   | THR | A | 421 | 10.831 | 22.035 | 67.585 | 1.00 | 30.99  |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
|    | ATOM | 3319 | O   | THR | A | 421 | 11.975 | 21.594 | 67.489 | 1.00 | 33.28 |
|    | ATOM | 3320 | CB  | THR | A | 421 | 10.394 | 23.969 | 69.166 | 1.00 | 21.94 |
|    | ATOM | 3321 | OG1 | THR | A | 421 | 10.567 | 25.369 | 69.263 | 1.00 | 24.52 |
| 5  | ATOM | 3322 | CG2 | THR | A | 421 | 11.399 | 23.221 | 70.045 | 1.00 | 20.12 |
|    | ATOM | 3323 | N   | ASP | A | 422 | 9.721  | 21.272 | 67.575 | 1.00 | 21.94 |
|    | ATOM | 3324 | CA  | ASP | A | 422 | 9.706  | 19.823 | 67.430 | 1.00 | 21.08 |
|    | ATOM | 3325 | C   | ASP | A | 422 | 10.323 | 19.401 | 66.104 | 1.00 | 31.16 |
|    | ATOM | 3326 | O   | ASP | A | 422 | 11.110 | 18.427 | 66.027 | 1.00 | 31.95 |
| 10 | ATOM | 3327 | CB  | ASP | A | 422 | 8.276  | 19.278 | 67.561 | 1.00 | 19.49 |
|    | ATOM | 3328 | CG  | ASP | A | 422 | 8.236  | 17.802 | 67.298 | 1.00 | 31.85 |
|    | ATOM | 3329 | OD1 | ASP | A | 422 | 9.130  | 17.040 | 67.654 | 1.00 | 29.73 |
|    | ATOM | 3330 | OD2 | ASP | A | 422 | 7.197  | 17.415 | 66.598 | 1.00 | 56.60 |
|    | ATOM | 3331 | N   | ASP | A | 423 | 9.957  | 20.146 | 65.049 | 1.00 | 26.75 |
| 15 | ATOM | 3332 | CA  | ASP | A | 423 | 10.505 | 19.876 | 63.729 | 1.00 | 26.01 |
|    | ATOM | 3333 | C   | ASP | A | 423 | 12.027 | 19.957 | 63.830 | 1.00 | 40.09 |
|    | ATOM | 3334 | O   | ASP | A | 423 | 12.753 | 19.020 | 63.500 | 1.00 | 47.09 |
|    | ATOM | 3335 | CB  | ASP | A | 423 | 10.000 | 20.833 | 62.631 | 1.00 | 24.86 |
|    | ATOM | 3336 | CG  | ASP | A | 423 | 8.538  | 20.722 | 62.343 | 1.00 | 39.90 |
| 20 | ATOM | 3337 | OD1 | ASP | A | 423 | 7.968  | 19.649 | 62.299 | 1.00 | 45.03 |
|    | ATOM | 3338 | OD2 | ASP | A | 423 | 7.943  | 21.887 | 62.113 | 1.00 | 40.43 |
|    | ATOM | 3339 | N   | TRP | A | 424 | 12.493 | 21.099 | 64.320 | 1.00 | 31.92 |
|    | ATOM | 3340 | CA  | TRP | A | 424 | 13.903 | 21.372 | 64.495 | 1.00 | 29.69 |
|    | ATOM | 3341 | C   | TRP | A | 424 | 14.611 | 20.271 | 65.282 | 1.00 | 33.81 |
| 25 | ATOM | 3342 | O   | TRP | A | 424 | 15.537 | 19.616 | 64.824 | 1.00 | 35.87 |
|    | ATOM | 3343 | CB  | TRP | A | 424 | 14.056 | 22.711 | 65.239 | 1.00 | 26.11 |
|    | ATOM | 3344 | CG  | TRP | A | 424 | 15.431 | 22.869 | 65.786 | 1.00 | 27.05 |
|    | ATOM | 3345 | CD1 | TRP | A | 424 | 16.518 | 23.302 | 65.101 | 1.00 | 29.65 |
|    | ATOM | 3346 | CD2 | TRP | A | 424 | 15.885 | 22.587 | 67.119 | 1.00 | 26.62 |
| 30 | ATOM | 3347 | NE1 | TRP | A | 424 | 17.612 | 23.321 | 65.922 | 1.00 | 27.83 |
|    | ATOM | 3348 | CE2 | TRP | A | 424 | 17.257 | 22.891 | 67.163 | 1.00 | 28.62 |
|    | ATOM | 3349 | CE3 | TRP | A | 424 | 15.260 | 22.138 | 68.269 | 1.00 | 29.69 |
|    | ATOM | 3350 | CZ2 | TRP | A | 424 | 18.010 | 22.758 | 68.319 | 1.00 | 29.28 |
| 35 | ATOM | 3351 | CZ3 | TRP | A | 424 | 16.000 | 21.993 | 69.429 | 1.00 | 33.50 |
|    | ATOM | 3352 | CH2 | TRP | A | 424 | 17.362 | 22.317 | 69.459 | 1.00 | 33.93 |
|    | ATOM | 3353 | N   | LYS | A | 425 | 14.156 | 20.090 | 66.497 | 1.00 | 28.75 |
|    | ATOM | 3354 | CA  | LYS | A | 425 | 14.723 | 19.105 | 67.373 | 1.00 | 29.43 |
|    | ATOM | 3355 | C   | LYS | A | 425 | 14.697 | 17.691 | 66.808 | 1.00 | 29.49 |
|    | ATOM | 3356 | O   | LYS | A | 425 | 15.627 | 16.928 | 67.030 | 1.00 | 27.65 |
| 40 | ATOM | 3357 | CB  | LYS | A | 425 | 14.078 | 19.171 | 68.744 | 1.00 | 29.70 |
|    | ATOM | 3358 | CG  | LYS | A | 425 | 14.860 | 18.414 | 69.787 | 1.00 | 28.11 |
|    | ATOM | 3359 | CD  | LYS | A | 425 | 14.161 | 18.409 | 71.132 | 1.00 | 23.57 |
|    | ATOM | 3360 | CE  | LYS | A | 425 | 14.300 | 17.063 | 71.815 | 1.00 | 36.16 |
| 45 | ATOM | 3361 | NZ  | LYS | A | 425 | 13.042 | 16.302 | 71.768 | 1.00 | 58.08 |
|    | ATOM | 3362 | N   | ASP | A | 426 | 13.606 | 17.361 | 66.107 | 1.00 | 19.05 |
|    | ATOM | 3363 | CA  | ASP | A | 426 | 13.417 | 16.070 | 65.516 | 1.00 | 18.43 |
|    | ATOM | 3364 | C   | ASP | A | 426 | 14.453 | 15.879 | 64.387 | 1.00 | 28.33 |
|    | ATOM | 3365 | O   | ASP | A | 426 | 15.070 | 14.832 | 64.232 | 1.00 | 31.25 |
| 50 | ATOM | 3366 | CB  | ASP | A | 426 | 11.920 | 15.840 | 65.098 | 1.00 | 19.79 |
|    | ATOM | 3367 | CG  | ASP | A | 426 | 10.998 | 15.575 | 66.274 | 1.00 | 25.54 |
|    | ATOM | 3368 | OD1 | ASP | A | 426 | 11.341 | 15.466 | 67.409 | 1.00 | 29.73 |
|    | ATOM | 3369 | OD2 | ASP | A | 426 | 9.804  | 15.611 | 65.938 | 1.00 | 20.67 |
|    | ATOM | 3370 | N   | PHE | A | 427 | 14.674 | 16.926 | 63.612 | 1.00 | 25.09 |
| 55 | ATOM | 3371 | CA  | PHE | A | 427 | 15.654 | 16.899 | 62.540 | 1.00 | 25.81 |
|    | ATOM | 3372 | C   | PHE | A | 427 | 17.066 | 16.718 | 63.159 | 1.00 | 34.01 |
|    | ATOM | 3373 | O   | PHE | A | 427 | 17.843 | 15.851 | 62.773 | 1.00 | 36.25 |
|    | ATOM | 3374 | CB  | PHE | A | 427 | 15.589 | 18.197 | 61.704 | 1.00 | 26.35 |
|    | ATOM | 3375 | CG  | PHE | A | 427 | 16.698 | 18.202 | 60.702 | 1.00 | 27.40 |
|    | ATOM | 3376 | CD1 | PHE | A | 427 | 16.714 | 17.247 | 59.686 | 1.00 | 29.97 |
| 60 | ATOM | 3377 | CD2 | PHE | A | 427 | 17.773 | 19.084 | 60.805 | 1.00 | 28.71 |
|    | ATOM | 3378 | CE1 | PHE | A | 427 | 17.730 | 17.194 | 58.733 | 1.00 | 27.72 |
|    | ATOM | 3379 | CE2 | PHE | A | 427 | 18.806 | 19.046 | 59.867 | 1.00 | 30.37 |
|    | ATOM | 3380 | CZ  | PHE | A | 427 | 18.780 | 18.104 | 58.837 | 1.00 | 26.34 |
|    | ATOM | 3381 | N   | LEU | A | 428 | 17.369 | 17.544 | 64.160 | 1.00 | 28.94 |
|    | ATOM | 3382 | CA  | LEU | A | 428 | 18.622 | 17.496 | 64.924 | 1.00 | 27.74 |



|    |      |      |     |     |   |     |        |        |        |      |        |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
|    | ATOM | 3383 | C   | LEU | A | 428 | 18.989 | 16.047 | 65.303 | 1.00 | 32.08  |
|    | ATOM | 3384 | O   | LEU | A | 428 | 20.145 | 15.647 | 65.209 | 1.00 | 36.38  |
|    | ATOM | 3385 | CB  | LEU | A | 428 | 18.510 | 18.362 | 66.223 | 1.00 | 24.68  |
| 5  | ATOM | 3386 | CG  | LEU | A | 428 | 19.778 | 18.377 | 67.079 | 1.00 | 24.30  |
|    | ATOM | 3387 | CD1 | LEU | A | 428 | 20.855 | 19.278 | 66.467 | 1.00 | 23.00  |
|    | ATOM | 3388 | CD2 | LEU | A | 428 | 19.446 | 18.856 | 68.481 | 1.00 | 16.41  |
|    | ATOM | 3389 | N   | TYR | A | 429 | 17.991 | 15.271 | 65.735 | 1.00 | 23.71  |
|    | ATOM | 3390 | CA  | TYR | A | 429 | 18.148 | 13.896 | 66.144 | 1.00 | 23.18  |
| 10 | ATOM | 3391 | C   | TYR | A | 429 | 18.311 | 12.967 | 64.976 | 1.00 | 26.62  |
|    | ATOM | 3392 | O   | TYR | A | 429 | 18.911 | 11.910 | 65.076 | 1.00 | 28.43  |
|    | ATOM | 3393 | CB  | TYR | A | 429 | 16.921 | 13.453 | 66.914 | 1.00 | 25.59  |
|    | ATOM | 3394 | CG  | TYR | A | 429 | 17.069 | 13.526 | 68.414 | 1.00 | 29.53  |
|    | ATOM | 3395 | CD1 | TYR | A | 429 | 16.823 | 14.714 | 69.114 | 1.00 | 31.11  |
|    | ATOM | 3396 | CD2 | TYR | A | 429 | 17.361 | 12.383 | 69.156 | 1.00 | 32.70  |
| 15 | ATOM | 3397 | CE1 | TYR | A | 429 | 16.916 | 14.769 | 70.510 | 1.00 | 32.23  |
|    | ATOM | 3398 | CE2 | TYR | A | 429 | 17.485 | 12.420 | 70.551 | 1.00 | 35.30  |
|    | ATOM | 3399 | CZ  | TYR | A | 429 | 17.251 | 13.623 | 71.231 | 1.00 | 41.02  |
|    | ATOM | 3400 | OH  | TYR | A | 429 | 17.339 | 13.679 | 72.609 | 1.00 | 30.02  |
| 20 | ATOM | 3401 | N   | SER | A | 430 | 17.748 | 13.342 | 63.854 | 1.00 | 21.68  |
|    | ATOM | 3402 | CA  | SER | A | 430 | 17.914 | 12.469 | 62.730 | 1.00 | 23.42  |
|    | ATOM | 3403 | C   | SER | A | 430 | 19.264 | 12.722 | 62.050 | 1.00 | 32.87  |
|    | ATOM | 3404 | O   | SER | A | 430 | 19.879 | 11.819 | 61.467 | 1.00 | 35.11  |
|    | ATOM | 3405 | CB  | SER | A | 430 | 16.756 | 12.541 | 61.773 | 1.00 | 28.79  |
| 25 | ATOM | 3406 | OG  | SER | A | 430 | 17.089 | 13.475 | 60.777 | 1.00 | 49.56  |
|    | ATOM | 3407 | N   | TYR | A | 431 | 19.748 | 13.955 | 62.132 | 1.00 | 27.18  |
|    | ATOM | 3408 | CA  | TYR | A | 431 | 21.017 | 14.296 | 61.537 | 1.00 | 27.14  |
|    | ATOM | 3409 | C   | TYR | A | 431 | 22.152 | 13.702 | 62.316 | 1.00 | 32.52  |
|    | ATOM | 3410 | O   | TYR | A | 431 | 23.155 | 13.242 | 61.771 | 1.00 | 33.64  |
| 30 | ATOM | 3411 | CB  | TYR | A | 431 | 21.216 | 15.818 | 61.385 | 1.00 | 31.07  |
|    | ATOM | 3412 | CG  | TYR | A | 431 | 22.566 | 16.265 | 60.812 | 1.00 | 35.63  |
|    | ATOM | 3413 | CD1 | TYR | A | 431 | 23.663 | 16.492 | 61.650 | 1.00 | 36.88  |
|    | ATOM | 3414 | CD2 | TYR | A | 431 | 22.735 | 16.496 | 59.444 | 1.00 | 36.92  |
|    | ATOM | 3415 | CE1 | TYR | A | 431 | 24.894 | 16.924 | 61.157 | 1.00 | 33.78  |
| 35 | ATOM | 3416 | CE2 | TYR | A | 431 | 23.964 | 16.916 | 58.924 | 1.00 | 37.86  |
|    | ATOM | 3417 | CZ  | TYR | A | 431 | 25.038 | 17.143 | 59.786 | 1.00 | 46.01  |
|    | ATOM | 3418 | OH  | TYR | A | 431 | 26.247 | 17.573 | 59.294 | 1.00 | 51.28  |
|    | ATOM | 3419 | N   | PHE | A | 432 | 21.964 | 13.728 | 63.606 | 1.00 | 29.66  |
|    | ATOM | 3420 | CA  | PHE | A | 432 | 22.939 | 13.215 | 64.526 | 1.00 | 29.12  |
| 40 | ATOM | 3421 | C   | PHE | A | 432 | 22.522 | 11.865 | 65.007 | 1.00 | 42.64  |
|    | ATOM | 3422 | O   | PHE | A | 432 | 22.499 | 11.593 | 66.197 | 1.00 | 46.77  |
|    | ATOM | 3423 | CB  | PHE | A | 432 | 23.063 | 14.157 | 65.719 | 1.00 | 30.24  |
|    | ATOM | 3424 | CG  | PHE | A | 432 | 23.962 | 15.327 | 65.401 | 1.00 | 33.03  |
|    | ATOM | 3425 | CD1 | PHE | A | 432 | 25.336 | 15.113 | 65.277 | 1.00 | 37.22  |
| 45 | ATOM | 3426 | CD2 | PHE | A | 432 | 23.470 | 16.624 | 65.232 | 1.00 | 30.70  |
|    | ATOM | 3427 | CE1 | PHE | A | 432 | 26.223 | 16.153 | 64.999 | 1.00 | 34.27  |
|    | ATOM | 3428 | CE2 | PHE | A | 432 | 24.349 | 17.667 | 64.938 | 1.00 | 31.71  |
|    | ATOM | 3429 | CZ  | PHE | A | 432 | 25.722 | 17.438 | 64.823 | 1.00 | 27.82  |
|    | ATOM | 3430 | N   | LYS | A | 433 | 22.174 | 11.029 | 64.063 | 1.00 | 42.50  |
| 50 | ATOM | 3431 | CA  | LYS | A | 433 | 21.669 | 9.670  | 64.270 | 1.00 | 40.87  |
|    | ATOM | 3432 | C   | LYS | A | 433 | 22.718 | 8.751  | 64.908 | 1.00 | 46.17  |
|    | ATOM | 3433 | O   | LYS | A | 433 | 22.405 | 7.734  | 65.513 | 1.00 | 48.48  |
|    | ATOM | 3434 | CB  | LYS | A | 433 | 21.245 | 9.106  | 62.917 | 1.00 | 39.25  |
|    | ATOM | 3435 | CG  | LYS | A | 433 | 19.988 | 8.241  | 63.017 | 1.00 | 84.17  |
| 55 | ATOM | 3436 | CD  | LYS | A | 433 | 18.925 | 8.660  | 62.000 | 1.00 | 100.00 |
|    | ATOM | 3437 | CE  | LYS | A | 433 | 17.523 | 8.172  | 62.384 | 1.00 | 100.00 |
|    | ATOM | 3438 | NZ  | LYS | A | 433 | 16.525 | 9.119  | 61.884 | 1.00 | 100.00 |
|    | ATOM | 3439 | N   | ASP | A | 434 | 24.002 | 9.112  | 64.697 | 1.00 | 45.20  |
|    | ATOM | 3440 | CA  | ASP | A | 434 | 25.083 | 8.349  | 65.321 | 1.00 | 47.80  |
| 60 | ATOM | 3441 | C   | ASP | A | 434 | 25.201 | 8.684  | 66.802 | 1.00 | 50.78  |
|    | ATOM | 3442 | O   | ASP | A | 434 | 25.474 | 7.845  | 67.653 | 1.00 | 55.76  |
|    | ATOM | 3443 | CB  | ASP | A | 434 | 26.405 | 8.567  | 64.562 | 1.00 | 53.91  |
|    | ATOM | 3444 | CG  | ASP | A | 434 | 26.123 | 8.474  | 63.069 | 1.00 | 93.32  |
|    | ATOM | 3445 | OD1 | ASP | A | 434 | 25.744 | 7.573  | 62.325 | 1.00 | 96.22  |
|    | ATOM | 3446 | OD2 | ASP | A | 434 | 26.119 | 9.664  | 62.753 | 1.00 | 100.00 |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
|    | ATOM | 3447 | N   | LYS | A | 435 | 25.015 | 9.978  | 67.085 | 1.00 | 38.82 |
|    | ATOM | 3448 | CA  | LYS | A | 435 | 24.974 | 10.404 | 68.468 | 1.00 | 34.57 |
|    | ATOM | 3449 | C   | LYS | A | 435 | 23.549 | 10.749 | 68.881 | 1.00 | 39.87 |
| 5  | ATOM | 3450 | O   | LYS | A | 435 | 23.070 | 11.840 | 68.693 | 1.00 | 40.34 |
|    | ATOM | 3451 | CB  | LYS | A | 435 | 25.864 | 11.631 | 68.615 | 1.00 | 34.69 |
|    | ATOM | 3452 | CG  | LYS | A | 435 | 27.064 | 11.595 | 67.679 | 1.00 | 40.86 |
|    | ATOM | 3453 | CD  | LYS | A | 435 | 27.703 | 12.975 | 67.532 | 1.00 | 51.04 |
|    | ATOM | 3454 | CE  | LYS | A | 435 | 29.242 | 12.904 | 67.557 | 1.00 | 24.08 |
| 10 | ATOM | 3455 | NZ  | LYS | A | 435 | 29.822 | 13.990 | 66.760 | 1.00 | 45.26 |
|    | ATOM | 3456 | N   | VAL | A | 436 | 22.843 | 9.728  | 69.414 | 1.00 | 38.07 |
|    | ATOM | 3457 | CA  | VAL | A | 436 | 21.601 | 10.036 | 70.111 | 1.00 | 36.86 |
|    | ATOM | 3458 | C   | VAL | A | 436 | 21.846 | 10.129 | 71.608 | 1.00 | 44.88 |
|    | ATOM | 3459 | O   | VAL | A | 436 | 21.289 | 10.948 | 72.300 | 1.00 | 46.42 |
| 15 | ATOM | 3460 | CB  | VAL | A | 436 | 20.567 | 8.923  | 69.816 | 1.00 | 37.37 |
|    | ATOM | 3461 | CG1 | VAL | A | 436 | 19.944 | 9.143  | 68.446 | 1.00 | 36.24 |
|    | ATOM | 3462 | CG2 | VAL | A | 436 | 21.227 | 7.556  | 69.854 | 1.00 | 36.80 |
|    | ATOM | 3463 | N   | ASP | A | 437 | 22.718 | 9.232  | 72.099 | 1.00 | 43.61 |
|    | ATOM | 3464 | CA  | ASP | A | 437 | 23.044 | 9.222  | 73.522 | 1.00 | 41.43 |
| 20 | ATOM | 3465 | C   | ASP | A | 437 | 23.657 | 10.546 | 73.958 | 1.00 | 45.71 |
|    | ATOM | 3466 | O   | ASP | A | 437 | 23.554 | 10.956 | 75.107 | 1.00 | 49.89 |
|    | ATOM | 3467 | CB  | ASP | A | 437 | 24.022 | 8.082  | 73.776 | 1.00 | 43.84 |
|    | ATOM | 3468 | CG  | ASP | A | 437 | 23.281 | 6.752  | 73.691 | 1.00 | 72.47 |
|    | ATOM | 3469 | OD1 | ASP | A | 437 | 22.062 | 6.769  | 73.823 | 1.00 | 74.64 |
| 25 | ATOM | 3470 | OD2 | ASP | A | 437 | 23.933 | 5.730  | 73.481 | 1.00 | 86.09 |
|    | ATOM | 3471 | N   | VAL | A | 438 | 24.333 | 11.324 | 73.122 | 1.00 | 40.21 |
|    | ATOM | 3472 | CA  | VAL | A | 438 | 24.807 | 12.624 | 73.577 | 1.00 | 40.97 |
|    | ATOM | 3473 | C   | VAL | A | 438 | 23.621 | 13.582 | 73.668 | 1.00 | 41.86 |
|    | ATOM | 3474 | O   | VAL | A | 438 | 23.368 | 14.276 | 74.657 | 1.00 | 39.95 |
| 30 | ATOM | 3475 | CB  | VAL | A | 438 | 25.875 | 13.165 | 72.615 | 1.00 | 47.47 |
|    | ATOM | 3476 | CG1 | VAL | A | 438 | 26.438 | 14.523 | 73.051 | 1.00 | 47.51 |
|    | ATOM | 3477 | CG2 | VAL | A | 438 | 26.996 | 12.149 | 72.440 | 1.00 | 47.51 |
|    | ATOM | 3478 | N   | LEU | A | 439 | 22.876 | 13.595 | 72.585 | 1.00 | 37.91 |
|    | ATOM | 3479 | CA  | LEU | A | 439 | 21.729 | 14.442 | 72.507 | 1.00 | 36.21 |
| 35 | ATOM | 3480 | C   | LEU | A | 439 | 20.850 | 14.190 | 73.695 | 1.00 | 40.03 |
|    | ATOM | 3481 | O   | LEU | A | 439 | 20.214 | 15.064 | 74.255 | 1.00 | 42.22 |
|    | ATOM | 3482 | CB  | LEU | A | 439 | 20.949 | 14.180 | 71.210 | 1.00 | 33.84 |
|    | ATOM | 3483 | CG  | LEU | A | 439 | 21.552 | 14.939 | 70.039 | 1.00 | 32.80 |
|    | ATOM | 3484 | CD1 | LEU | A | 439 | 20.813 | 14.538 | 68.775 | 1.00 | 34.08 |
| 40 | ATOM | 3485 | CD2 | LEU | A | 439 | 21.435 | 16.434 | 70.258 | 1.00 | 23.80 |
|    | ATOM | 3486 | N   | ASN | A | 440 | 20.810 | 12.953 | 74.076 | 1.00 | 34.03 |
|    | ATOM | 3487 | CA  | ASN | A | 440 | 19.971 | 12.603 | 75.187 | 1.00 | 34.00 |
|    | ATOM | 3488 | C   | ASN | A | 440 | 20.494 | 13.093 | 76.532 | 1.00 | 40.95 |
|    | ATOM | 3489 | O   | ASN | A | 440 | 19.816 | 12.995 | 77.544 | 1.00 | 42.09 |
| 45 | ATOM | 3490 | CB  | ASN | A | 440 | 19.681 | 11.095 | 75.178 | 1.00 | 24.89 |
|    | ATOM | 3491 | CG  | ASN | A | 440 | 18.790 | 10.635 | 74.028 | 1.00 | 46.52 |
|    | ATOM | 3492 | OD1 | ASN | A | 440 | 19.005 | 9.537  | 73.480 | 1.00 | 58.82 |
|    | ATOM | 3493 | ND2 | ASN | A | 440 | 17.769 | 11.440 | 73.680 | 1.00 | 31.11 |
|    | ATOM | 3494 | N   | GLN | A | 441 | 21.707 | 13.623 | 76.531 | 1.00 | 36.98 |
| 50 | ATOM | 3495 | CA  | GLN | A | 441 | 22.339 | 14.095 | 77.744 | 1.00 | 35.47 |
|    | ATOM | 3496 | C   | GLN | A | 441 | 21.879 | 15.478 | 78.067 | 1.00 | 36.00 |
|    | ATOM | 3497 | O   | GLN | A | 441 | 22.137 | 16.029 | 79.142 | 1.00 | 34.96 |
|    | ATOM | 3498 | CB  | GLN | A | 441 | 23.878 | 14.109 | 77.581 | 1.00 | 38.10 |
|    | ATOM | 3499 | CG  | GLN | A | 441 | 24.504 | 12.692 | 77.422 | 1.00 | 52.06 |
| 55 | ATOM | 3500 | CD  | GLN | A | 441 | 25.954 | 12.730 | 76.955 | 1.00 | 81.69 |
|    | ATOM | 3501 | OE1 | GLN | A | 441 | 26.476 | 13.796 | 76.609 | 1.00 | 74.46 |
|    | ATOM | 3502 | NE2 | GLN | A | 441 | 26.616 | 11.574 | 76.972 | 1.00 | 91.09 |
|    | ATOM | 3503 | N   | VAL | A | 442 | 21.197 | 16.067 | 77.112 | 1.00 | 31.86 |
|    | ATOM | 3504 | CA  | VAL | A | 442 | 20.753 | 17.411 | 77.384 | 1.00 | 32.78 |
|    | ATOM | 3505 | C   | VAL | A | 442 | 19.354 | 17.468 | 77.970 | 1.00 | 38.24 |
| 60 | ATOM | 3506 | O   | VAL | A | 442 | 18.468 | 16.700 | 77.588 | 1.00 | 42.83 |
|    | ATOM | 3507 | CB  | VAL | A | 442 | 20.845 | 18.277 | 76.159 | 1.00 | 34.84 |
|    | ATOM | 3508 | CG1 | VAL | A | 442 | 21.430 | 17.435 | 75.020 | 1.00 | 34.65 |
|    | ATOM | 3509 | CG2 | VAL | A | 442 | 19.441 | 18.705 | 75.811 | 1.00 | 33.21 |
|    | ATOM | 3510 | N   | ASP | A | 443 | 19.172 | 18.388 | 78.908 | 1.00 | 25.60 |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
|    | ATOM | 3511 | CA  | ASP | A | 443 | 17.931 | 18.634 | 79.616 | 1.00 | 24.57 |
|    | ATOM | 3512 | C   | ASP | A | 443 | 16.996 | 19.533 | 78.791 | 1.00 | 32.14 |
|    | ATOM | 3513 | O   | ASP | A | 443 | 16.744 | 20.732 | 79.073 | 1.00 | 34.77 |
| 5  | ATOM | 3514 | CB  | ASP | A | 443 | 18.332 | 19.272 | 80.957 | 1.00 | 27.11 |
|    | ATOM | 3515 | CG  | ASP | A | 443 | 17.216 | 19.413 | 81.901 | 1.00 | 39.99 |
|    | ATOM | 3516 | OD1 | ASP | A | 443 | 16.063 | 19.234 | 81.573 | 1.00 | 44.78 |
|    | ATOM | 3517 | OD2 | ASP | A | 443 | 17.631 | 19.753 | 83.094 | 1.00 | 56.66 |
|    | ATOM | 3518 | N   | TRP | A | 444 | 16.525 | 18.914 | 77.722 | 1.00 | 28.30 |
| 10 | ATOM | 3519 | CA  | TRP | A | 444 | 15.614 | 19.507 | 76.757 | 1.00 | 26.27 |
|    | ATOM | 3520 | C   | TRP | A | 444 | 14.460 | 20.296 | 77.416 | 1.00 | 31.52 |
|    | ATOM | 3521 | O   | TRP | A | 444 | 14.102 | 21.409 | 76.988 | 1.00 | 34.63 |
|    | ATOM | 3522 | CB  | TRP | A | 444 | 15.067 | 18.398 | 75.799 | 1.00 | 21.47 |
|    | ATOM | 3523 | CG  | TRP | A | 444 | 16.095 | 17.951 | 74.806 | 1.00 | 22.03 |
| 15 | ATOM | 3524 | CD1 | TRP | A | 444 | 16.675 | 16.718 | 74.736 | 1.00 | 25.16 |
|    | ATOM | 3525 | CD2 | TRP | A | 444 | 16.733 | 18.738 | 73.776 | 1.00 | 20.36 |
|    | ATOM | 3526 | NE1 | TRP | A | 444 | 17.623 | 16.677 | 73.738 | 1.00 | 23.97 |
|    | ATOM | 3527 | CE2 | TRP | A | 444 | 17.688 | 17.906 | 73.138 | 1.00 | 24.71 |
|    | ATOM | 3528 | CE3 | TRP | A | 444 | 16.596 | 20.045 | 73.342 | 1.00 | 20.86 |
| 20 | ATOM | 3529 | CZ2 | TRP | A | 444 | 18.448 | 18.345 | 72.060 | 1.00 | 24.51 |
|    | ATOM | 3530 | CZ3 | TRP | A | 444 | 17.353 | 20.471 | 72.264 | 1.00 | 22.88 |
|    | ATOM | 3531 | CH2 | TRP | A | 444 | 18.281 | 19.643 | 71.643 | 1.00 | 23.48 |
|    | ATOM | 3532 | N   | ASN | A | 445 | 13.855 | 19.711 | 78.457 | 1.00 | 24.92 |
|    | ATOM | 3533 | CA  | ASN | A | 445 | 12.723 | 20.326 | 79.113 | 1.00 | 26.30 |
| 25 | ATOM | 3534 | C   | ASN | A | 445 | 13.040 | 21.677 | 79.729 | 1.00 | 30.17 |
|    | ATOM | 3535 | O   | ASN | A | 445 | 12.291 | 22.660 | 79.547 | 1.00 | 31.86 |
|    | ATOM | 3536 | CB  | ASN | A | 445 | 11.987 | 19.382 | 80.094 | 1.00 | 40.83 |
|    | ATOM | 3537 | CG  | ASN | A | 445 | 10.946 | 20.033 | 81.020 | 1.00 | 87.07 |
|    | ATOM | 3538 | OD1 | ASN | A | 445 | 11.271 | 20.635 | 82.065 | 1.00 | 86.38 |
| 30 | ATOM | 3539 | ND2 | ASN | A | 445 | 9.670  | 19.848 | 80.688 | 1.00 | 71.65 |
|    | ATOM | 3540 | N   | ALA | A | 446 | 14.147 | 21.687 | 80.436 | 1.00 | 22.70 |
|    | ATOM | 3541 | CA  | ALA | A | 446 | 14.583 | 22.886 | 81.073 | 1.00 | 24.45 |
|    | ATOM | 3542 | C   | ALA | A | 446 | 14.886 | 23.896 | 79.990 | 1.00 | 30.52 |
|    | ATOM | 3543 | O   | ALA | A | 446 | 14.324 | 25.001 | 79.936 | 1.00 | 33.92 |
| 35 | ATOM | 3544 | CB  | ALA | A | 446 | 15.814 | 22.543 | 81.900 | 1.00 | 25.68 |
|    | ATOM | 3545 | N   | TRP | A | 447 | 15.776 | 23.494 | 79.102 | 1.00 | 25.24 |
|    | ATOM | 3546 | CA  | TRP | A | 447 | 16.162 | 24.384 | 78.034 | 1.00 | 26.83 |
|    | ATOM | 3547 | C   | TRP | A | 447 | 14.989 | 24.912 | 77.223 | 1.00 | 31.32 |
|    | ATOM | 3548 | O   | TRP | A | 447 | 14.971 | 26.089 | 76.875 | 1.00 | 30.48 |
| 40 | ATOM | 3549 | CB  | TRP | A | 447 | 17.166 | 23.725 | 77.062 | 1.00 | 25.78 |
|    | ATOM | 3550 | CG  | TRP | A | 447 | 18.625 | 23.815 | 77.421 | 1.00 | 26.60 |
|    | ATOM | 3551 | CD1 | TRP | A | 447 | 19.343 | 22.840 | 78.046 | 1.00 | 28.89 |
|    | ATOM | 3552 | CD2 | TRP | A | 447 | 19.554 | 24.896 | 77.165 | 1.00 | 26.16 |
|    | ATOM | 3553 | NE1 | TRP | A | 447 | 20.654 | 23.217 | 78.197 | 1.00 | 27.23 |
| 45 | ATOM | 3554 | CE2 | TRP | A | 447 | 20.822 | 24.476 | 77.660 | 1.00 | 29.00 |
|    | ATOM | 3555 | CE3 | TRP | A | 447 | 19.435 | 26.162 | 76.607 | 1.00 | 27.56 |
|    | ATOM | 3556 | CZ2 | TRP | A | 447 | 21.954 | 25.290 | 77.583 | 1.00 | 27.95 |
|    | ATOM | 3557 | CZ3 | TRP | A | 447 | 20.554 | 26.966 | 76.538 | 1.00 | 29.93 |
|    | ATOM | 3558 | CH2 | TRP | A | 447 | 21.792 | 26.539 | 77.035 | 1.00 | 30.16 |
| 50 | ATOM | 3559 | N   | LEU | A | 448 | 14.029 | 24.034 | 76.893 | 1.00 | 26.54 |
|    | ATOM | 3560 | CA  | LEU | A | 448 | 12.896 | 24.421 | 76.052 | 1.00 | 26.92 |
|    | ATOM | 3561 | C   | LEU | A | 448 | 11.734 | 25.064 | 76.779 | 1.00 | 36.15 |
|    | ATOM | 3562 | O   | LEU | A | 448 | 11.089 | 26.031 | 76.304 | 1.00 | 31.19 |
|    | ATOM | 3563 | CB  | LEU | A | 448 | 12.338 | 23.197 | 75.307 | 1.00 | 25.26 |
| 55 | ATOM | 3564 | CG  | LEU | A | 448 | 13.311 | 22.545 | 74.332 | 1.00 | 28.29 |
|    | ATOM | 3565 | CD1 | LEU | A | 448 | 12.597 | 21.455 | 73.530 | 1.00 | 30.49 |
|    | ATOM | 3566 | CD2 | LEU | A | 448 | 13.879 | 23.576 | 73.375 | 1.00 | 21.94 |
|    | ATOM | 3567 | N   | TYR | A | 449 | 11.472 | 24.455 | 77.924 | 1.00 | 33.14 |
|    | ATOM | 3568 | CA  | TYR | A | 449 | 10.373 | 24.835 | 78.747 | 1.00 | 30.64 |
| 60 | ATOM | 3569 | C   | TYR | A | 449 | 10.646 | 25.525 | 80.041 | 1.00 | 34.31 |
|    | ATOM | 3570 | O   | TYR | A | 449 | 9.750  | 26.191 | 80.529 | 1.00 | 41.98 |
|    | ATOM | 3571 | CB  | TYR | A | 449 | 9.400  | 23.674 | 78.916 | 1.00 | 29.14 |
|    | ATOM | 3572 | CG  | TYR | A | 449 | 9.212  | 23.089 | 77.556 | 1.00 | 26.50 |
|    | ATOM | 3573 | CD1 | TYR | A | 449 | 8.762  | 23.869 | 76.485 | 1.00 | 24.36 |
|    | ATOM | 3574 | CD2 | TYR | A | 449 | 9.560  | 21.762 | 77.325 | 1.00 | 28.48 |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
|    | ATOM | 3575 | CE1 | TYR | A | 449 | 8.626  | 23.331 | 75.202 | 1.00 | 17.56 |
|    | ATOM | 3576 | CE2 | TYR | A | 449 | 9.427  | 21.205 | 76.054 | 1.00 | 29.93 |
|    | ATOM | 3577 | CZ  | TYR | A | 449 | 8.959  | 21.988 | 74.998 | 1.00 | 33.65 |
| 5  | ATOM | 3578 | OH  | TYR | A | 449 | 8.840  | 21.415 | 73.762 | 1.00 | 39.47 |
|    | ATOM | 3579 | N   | SER | A | 450 | 11.806 | 25.413 | 80.644 | 1.00 | 22.72 |
|    | ATOM | 3580 | CA  | SER | A | 450 | 11.902 | 26.149 | 81.900 | 1.00 | 21.21 |
|    | ATOM | 3581 | C   | SER | A | 450 | 12.278 | 27.625 | 81.749 | 1.00 | 23.98 |
|    | ATOM | 3582 | O   | SER | A | 450 | 12.966 | 28.035 | 80.810 | 1.00 | 27.17 |
| 10 | ATOM | 3583 | CB  | SER | A | 450 | 12.666 | 25.436 | 83.010 | 1.00 | 24.83 |
|    | ATOM | 3584 | OG  | SER | A | 450 | 12.540 | 24.046 | 82.871 | 1.00 | 36.29 |
|    | ATOM | 3585 | N   | PRO | A | 451 | 11.806 | 28.430 | 82.689 | 1.00 | 19.76 |
|    | ATOM | 3586 | CA  | PRO | A | 451 | 12.111 | 29.840 | 82.669 | 1.00 | 18.20 |
|    | ATOM | 3587 | C   | PRO | A | 451 | 13.461 | 29.988 | 83.271 | 1.00 | 21.72 |
| 15 | ATOM | 3588 | O   | PRO | A | 451 | 14.022 | 29.015 | 83.742 | 1.00 | 24.34 |
|    | ATOM | 3589 | CB  | PRO | A | 451 | 11.185 | 30.485 | 83.695 | 1.00 | 18.85 |
|    | ATOM | 3590 | CG  | PRO | A | 451 | 10.836 | 29.390 | 84.677 | 1.00 | 23.13 |
|    | ATOM | 3591 | CD  | PRO | A | 451 | 11.002 | 28.078 | 83.900 | 1.00 | 19.61 |
|    | ATOM | 3592 | N   | GLY | A | 452 | 13.959 | 31.212 | 83.307 | 1.00 | 18.97 |
| 20 | ATOM | 3593 | CA  | GLY | A | 452 | 15.241 | 31.444 | 83.922 | 1.00 | 19.09 |
|    | ATOM | 3594 | C   | GLY | A | 452 | 16.382 | 31.107 | 83.016 | 1.00 | 26.20 |
|    | ATOM | 3595 | O   | GLY | A | 452 | 16.191 | 30.916 | 81.819 | 1.00 | 27.37 |
|    | ATOM | 3596 | N   | LEU | A | 453 | 17.557 | 31.057 | 83.650 | 1.00 | 25.48 |
|    | ATOM | 3597 | CA  | LEU | A | 453 | 18.843 | 30.750 | 83.029 | 1.00 | 25.32 |
| 25 | ATOM | 3598 | C   | LEU | A | 453 | 18.906 | 29.322 | 82.629 | 1.00 | 26.21 |
|    | ATOM | 3599 | O   | LEU | A | 453 | 18.400 | 28.458 | 83.322 | 1.00 | 25.04 |
|    | ATOM | 3600 | CB  | LEU | A | 453 | 20.042 | 31.119 | 83.938 | 1.00 | 25.46 |
|    | ATOM | 3601 | CG  | LEU | A | 453 | 20.280 | 32.632 | 83.904 | 1.00 | 31.82 |
|    | ATOM | 3602 | CD1 | LEU | A | 453 | 21.019 | 33.087 | 85.119 | 1.00 | 31.78 |
| 30 | ATOM | 3603 | CD2 | LEU | A | 453 | 21.046 | 33.056 | 82.651 | 1.00 | 41.50 |
|    | ATOM | 3604 | N   | PRO | A | 454 | 19.510 | 29.082 | 81.489 | 1.00 | 22.97 |
|    | ATOM | 3605 | CA  | PRO | A | 454 | 19.585 | 27.747 | 81.003 | 1.00 | 21.60 |
|    | ATOM | 3606 | C   | PRO | A | 454 | 20.145 | 26.890 | 82.075 | 1.00 | 26.94 |
|    | ATOM | 3607 | O   | PRO | A | 454 | 20.923 | 27.359 | 82.893 | 1.00 | 29.09 |
| 35 | ATOM | 3608 | CB  | PRO | A | 454 | 20.489 | 27.780 | 79.768 | 1.00 | 22.34 |
|    | ATOM | 3609 | CG  | PRO | A | 454 | 20.777 | 29.232 | 79.470 | 1.00 | 23.69 |
|    | ATOM | 3610 | CD  | PRO | A | 454 | 20.136 | 30.054 | 80.556 | 1.00 | 20.82 |
|    | ATOM | 3611 | N   | PRO | A | 455 | 19.721 | 25.648 | 82.067 | 1.00 | 25.61 |
|    | ATOM | 3612 | CA  | PRO | A | 455 | 20.167 | 24.683 | 83.031 | 1.00 | 24.27 |
| 40 | ATOM | 3613 | C   | PRO | A | 455 | 21.661 | 24.568 | 82.991 | 1.00 | 30.95 |
|    | ATOM | 3614 | O   | PRO | A | 455 | 22.225 | 24.062 | 83.920 | 1.00 | 33.47 |
|    | ATOM | 3615 | CB  | PRO | A | 455 | 19.631 | 23.320 | 82.592 | 1.00 | 25.04 |
|    | ATOM | 3616 | CG  | PRO | A | 455 | 19.149 | 23.497 | 81.162 | 1.00 | 33.02 |
|    | ATOM | 3617 | CD  | PRO | A | 455 | 19.111 | 25.005 | 80.888 | 1.00 | 28.49 |
| 45 | ATOM | 3618 | N   | ILE | A | 456 | 22.305 | 25.002 | 81.911 | 1.00 | 27.91 |
|    | ATOM | 3619 | CA  | ILE | A | 456 | 23.764 | 24.893 | 81.821 | 1.00 | 27.82 |
|    | ATOM | 3620 | C   | ILE | A | 456 | 24.395 | 26.057 | 81.077 | 1.00 | 34.73 |
|    | ATOM | 3621 | O   | ILE | A | 456 | 23.737 | 26.769 | 80.293 | 1.00 | 37.01 |
|    | ATOM | 3622 | CB  | ILE | A | 456 | 24.228 | 23.540 | 81.259 | 1.00 | 31.34 |
| 50 | ATOM | 3623 | CG1 | ILE | A | 456 | 25.721 | 23.305 | 81.417 | 1.00 | 29.78 |
|    | ATOM | 3624 | CG2 | ILE | A | 456 | 23.865 | 23.369 | 79.788 | 1.00 | 32.96 |
|    | ATOM | 3625 | CD1 | ILE | A | 456 | 26.054 | 21.852 | 81.116 | 1.00 | 23.94 |
|    | ATOM | 3626 | N   | LYS | A | 457 | 25.680 | 26.252 | 81.334 | 1.00 | 30.52 |
|    | ATOM | 3627 | CA  | LYS | A | 457 | 26.405 | 27.335 | 80.707 | 1.00 | 30.21 |
| 55 | ATOM | 3628 | C   | LYS | A | 457 | 27.515 | 26.808 | 79.835 | 1.00 | 32.14 |
|    | ATOM | 3629 | O   | LYS | A | 457 | 28.328 | 26.037 | 80.273 | 1.00 | 33.07 |
|    | ATOM | 3630 | CB  | LYS | A | 457 | 26.953 | 28.264 | 81.749 | 1.00 | 32.38 |
|    | ATOM | 3631 | CG  | LYS | A | 457 | 27.818 | 29.327 | 81.121 | 1.00 | 34.64 |
|    | ATOM | 3632 | CD  | LYS | A | 457 | 28.288 | 30.306 | 82.166 | 1.00 | 13.41 |
| 60 | ATOM | 3633 | CE  | LYS | A | 457 | 28.803 | 31.596 | 81.565 | 1.00 | 18.04 |
|    | ATOM | 3634 | NZ  | LYS | A | 457 | 28.974 | 32.643 | 82.595 | 1.00 | 26.77 |
|    | ATOM | 3635 | N   | PRO | A | 458 | 27.567 | 27.208 | 78.589 | 1.00 | 27.50 |
|    | ATOM | 3636 | CA  | PRO | A | 458 | 28.630 | 26.675 | 77.737 | 1.00 | 26.85 |
|    | ATOM | 3637 | C   | PRO | A | 458 | 29.994 | 27.147 | 78.185 | 1.00 | 26.89 |
|    | ATOM | 3638 | O   | PRO | A | 458 | 30.128 | 27.876 | 79.167 | 1.00 | 24.86 |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
|    | ATOM | 3639 | CB  | PRO | A | 458 | 28.335 | 27.191 | 76.316 | 1.00 | 29.41 |
|    | ATOM | 3640 | CG  | PRO | A | 458 | 26.952 | 27.864 | 76.375 | 1.00 | 33.24 |
|    | ATOM | 3641 | CD  | PRO | A | 458 | 26.574 | 28.044 | 77.848 | 1.00 | 26.12 |
| 5  | ATOM | 3642 | N   | ASN | A | 459 | 31.005 | 26.754 | 77.440 | 1.00 | 22.13 |
|    | ATOM | 3643 | CA  | ASN | A | 459 | 32.359 | 27.191 | 77.735 | 1.00 | 22.29 |
|    | ATOM | 3644 | C   | ASN | A | 459 | 32.751 | 28.325 | 76.820 | 1.00 | 30.27 |
|    | ATOM | 3645 | O   | ASN | A | 459 | 32.451 | 28.296 | 75.617 | 1.00 | 32.89 |
|    | ATOM | 3646 | CB  | ASN | A | 459 | 33.315 | 26.060 | 77.494 | 1.00 | 25.03 |
| 10 | ATOM | 3647 | CG  | ASN | A | 459 | 32.766 | 24.846 | 78.155 | 1.00 | 49.54 |
|    | ATOM | 3648 | OD1 | ASN | A | 459 | 32.618 | 24.822 | 79.383 | 1.00 | 50.09 |
|    | ATOM | 3649 | ND2 | ASN | A | 459 | 32.411 | 23.870 | 77.332 | 1.00 | 38.39 |
|    | ATOM | 3650 | N   | TYR | A | 460 | 33.448 | 29.316 | 77.380 | 1.00 | 25.58 |
|    | ATOM | 3651 | CA  | TYR | A | 460 | 33.851 | 30.493 | 76.625 | 1.00 | 23.89 |
| 15 | ATOM | 3652 | C   | TYR | A | 460 | 35.298 | 30.853 | 76.745 | 1.00 | 34.20 |
|    | ATOM | 3653 | O   | TYR | A | 460 | 35.849 | 30.862 | 77.839 | 1.00 | 35.27 |
|    | ATOM | 3654 | CB  | TYR | A | 460 | 33.120 | 31.708 | 77.171 | 1.00 | 24.38 |
|    | ATOM | 3655 | CG  | TYR | A | 460 | 31.636 | 31.631 | 77.024 | 1.00 | 26.98 |
|    | ATOM | 3656 | CD1 | TYR | A | 460 | 31.029 | 32.011 | 75.829 | 1.00 | 30.69 |
| 20 | ATOM | 3657 | CD2 | TYR | A | 460 | 30.838 | 31.168 | 78.064 | 1.00 | 25.70 |
|    | ATOM | 3658 | CE1 | TYR | A | 460 | 29.644 | 31.952 | 75.684 | 1.00 | 28.77 |
|    | ATOM | 3659 | CE2 | TYR | A | 460 | 29.453 | 31.096 | 77.938 | 1.00 | 25.24 |
|    | ATOM | 3660 | CZ  | TYR | A | 460 | 28.863 | 31.496 | 76.741 | 1.00 | 24.49 |
|    | ATOM | 3661 | OH  | TYR | A | 460 | 27.519 | 31.443 | 76.587 | 1.00 | 28.39 |
| 25 | ATOM | 3662 | N   | ASP | A | 461 | 35.893 | 31.227 | 75.616 | 1.00 | 30.58 |
|    | ATOM | 3663 | CA  | ASP | A | 461 | 37.268 | 31.640 | 75.654 | 1.00 | 27.51 |
|    | ATOM | 3664 | C   | ASP | A | 461 | 37.319 | 32.941 | 76.464 | 1.00 | 23.53 |
|    | ATOM | 3665 | O   | ASP | A | 461 | 36.377 | 33.704 | 76.396 | 1.00 | 26.62 |
|    | ATOM | 3666 | CB  | ASP | A | 461 | 37.821 | 31.784 | 74.218 | 1.00 | 27.30 |
| 30 | ATOM | 3667 | CG  | ASP | A | 461 | 39.137 | 32.466 | 74.260 | 1.00 | 32.53 |
|    | ATOM | 3668 | OD1 | ASP | A | 461 | 39.262 | 33.672 | 74.334 | 1.00 | 39.66 |
|    | ATOM | 3669 | OD2 | ASP | A | 461 | 40.130 | 31.628 | 74.306 | 1.00 | 44.34 |
|    | ATOM | 3670 | N   | MET | A | 462 | 38.375 | 33.234 | 77.224 | 1.00 | 17.26 |
|    | ATOM | 3671 | CA  | MET | A | 462 | 38.396 | 34.511 | 78.008 | 1.00 | 18.66 |
| 35 | ATOM | 3672 | C   | MET | A | 462 | 39.299 | 35.634 | 77.485 | 1.00 | 24.02 |
|    | ATOM | 3673 | O   | MET | A | 462 | 39.336 | 36.738 | 78.011 | 1.00 | 24.56 |
|    | ATOM | 3674 | CB  | MET | A | 462 | 38.818 | 34.186 | 79.431 | 1.00 | 22.99 |
|    | ATOM | 3675 | CG  | MET | A | 462 | 37.808 | 33.209 | 80.025 | 1.00 | 28.98 |
|    | ATOM | 3676 | SD  | MET | A | 462 | 36.166 | 33.969 | 79.951 | 1.00 | 33.22 |
| 40 | ATOM | 3677 | CE  | MET | A | 462 | 36.420 | 35.300 | 81.153 | 1.00 | 27.89 |
|    | ATOM | 3678 | N   | THR | A | 463 | 40.067 | 35.348 | 76.461 | 1.00 | 22.57 |
|    | ATOM | 3679 | CA  | THR | A | 463 | 41.015 | 36.285 | 75.911 | 1.00 | 22.64 |
|    | ATOM | 3680 | C   | THR | A | 463 | 40.690 | 37.738 | 75.961 | 1.00 | 33.12 |
|    | ATOM | 3681 | O   | THR | A | 463 | 41.372 | 38.493 | 76.640 | 1.00 | 35.27 |
| 45 | ATOM | 3682 | CB  | THR | A | 463 | 41.574 | 35.929 | 74.536 | 1.00 | 29.80 |
|    | ATOM | 3683 | OG1 | THR | A | 463 | 41.939 | 34.576 | 74.509 | 1.00 | 26.74 |
|    | ATOM | 3684 | CG2 | THR | A | 463 | 42.797 | 36.793 | 74.224 | 1.00 | 18.79 |
|    | ATOM | 3685 | N   | LEU | A | 464 | 39.700 | 38.141 | 75.177 | 1.00 | 30.50 |
|    | ATOM | 3686 | CA  | LEU | A | 464 | 39.293 | 39.533 | 75.061 | 1.00 | 29.15 |
| 50 | ATOM | 3687 | C   | LEU | A | 464 | 38.490 | 40.067 | 76.216 | 1.00 | 34.24 |
|    | ATOM | 3688 | O   | LEU | A | 464 | 38.439 | 41.270 | 76.422 | 1.00 | 37.12 |
|    | ATOM | 3689 | CB  | LEU | A | 464 | 38.537 | 39.767 | 73.743 | 1.00 | 29.20 |
|    | ATOM | 3690 | CG  | LEU | A | 464 | 39.393 | 39.394 | 72.527 | 1.00 | 33.73 |
|    | ATOM | 3691 | CD1 | LEU | A | 464 | 38.609 | 39.565 | 71.217 | 1.00 | 32.72 |
| 55 | ATOM | 3692 | CD2 | LEU | A | 464 | 40.648 | 40.261 | 72.499 | 1.00 | 26.22 |
|    | ATOM | 3693 | N   | THR | A | 465 | 37.855 | 39.167 | 76.964 | 1.00 | 30.71 |
|    | ATOM | 3694 | CA  | THR | A | 465 | 37.005 | 39.496 | 78.103 | 1.00 | 28.58 |
|    | ATOM | 3695 | C   | THR | A | 465 | 37.800 | 39.893 | 79.324 | 1.00 | 30.69 |
|    | ATOM | 3696 | O   | THR | A | 465 | 37.530 | 40.865 | 80.030 | 1.00 | 31.27 |
| 60 | ATOM | 3697 | CB  | THR | A | 465 | 36.016 | 38.328 | 78.372 | 1.00 | 35.85 |
|    | ATOM | 3698 | OG1 | THR | A | 465 | 35.101 | 38.212 | 77.296 | 1.00 | 50.93 |
|    | ATOM | 3699 | CG2 | THR | A | 465 | 35.255 | 38.451 | 79.690 | 1.00 | 26.34 |
|    | ATOM | 3700 | N   | ASN | A | 466 | 38.802 | 39.111 | 79.568 | 1.00 | 24.40 |
|    | ATOM | 3701 | CA  | ASN | A | 466 | 39.635 | 39.375 | 80.688 | 1.00 | 23.11 |
|    | ATOM | 3702 | C   | ASN | A | 466 | 39.899 | 40.856 | 80.967 | 1.00 | 28.37 |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
|    | ATOM | 3703 | O   | ASN | A | 466 | 39.763 | 41.270 | 82.120 | 1.00 | 27.03 |
|    | ATOM | 3704 | CB  | ASN | A | 466 | 40.921 | 38.543 | 80.629 | 1.00 | 20.30 |
|    | ATOM | 3705 | CG  | ASN | A | 466 | 40.709 | 37.145 | 81.155 | 1.00 | 32.26 |
| 5  | ATOM | 3706 | OD1 | ASN | A | 466 | 41.384 | 36.191 | 80.723 | 1.00 | 29.29 |
|    | ATOM | 3707 | ND2 | ASN | A | 466 | 39.775 | 37.015 | 82.111 | 1.00 | 28.19 |
|    | ATOM | 3708 | N   | ALA | A | 467 | 40.306 | 41.666 | 79.967 | 1.00 | 27.97 |
|    | ATOM | 3709 | CA  | ALA | A | 467 | 40.587 | 43.079 | 80.295 | 1.00 | 26.66 |
|    | ATOM | 3710 | C   | ALA | A | 467 | 39.352 | 43.827 | 80.720 | 1.00 | 31.78 |
| 10 | ATOM | 3711 | O   | ALA | A | 467 | 39.406 | 44.845 | 81.393 | 1.00 | 31.71 |
|    | ATOM | 3712 | CB  | ALA | A | 467 | 41.365 | 43.837 | 79.256 | 1.00 | 25.99 |
|    | ATOM | 3713 | N   | CYS | A | 468 | 38.217 | 43.277 | 80.336 | 1.00 | 28.06 |
|    | ATOM | 3714 | CA  | CYS | A | 468 | 36.942 | 43.862 | 80.693 | 1.00 | 25.80 |
|    | ATOM | 3715 | C   | CYS | A | 468 | 36.668 | 43.619 | 82.165 | 1.00 | 26.47 |
| 15 | ATOM | 3716 | O   | CYS | A | 468 | 36.469 | 44.517 | 82.963 | 1.00 | 27.99 |
|    | ATOM | 3717 | CB  | CYS | A | 468 | 35.882 | 43.376 | 79.696 | 1.00 | 24.56 |
|    | ATOM | 3718 | SG  | CYS | A | 468 | 36.455 | 43.873 | 78.049 | 1.00 | 27.76 |
|    | ATOM | 3719 | N   | ILE | A | 469 | 36.752 | 42.384 | 82.540 | 1.00 | 24.34 |
|    | ATOM | 3720 | CA  | ILE | A | 469 | 36.599 | 42.052 | 83.921 | 1.00 | 25.23 |
| 20 | ATOM | 3721 | C   | ILE | A | 469 | 37.560 | 42.800 | 84.876 | 1.00 | 28.13 |
|    | ATOM | 3722 | O   | ILE | A | 469 | 37.175 | 43.220 | 85.950 | 1.00 | 29.54 |
|    | ATOM | 3723 | CB  | ILE | A | 469 | 36.858 | 40.574 | 84.068 | 1.00 | 27.23 |
|    | ATOM | 3724 | CG1 | ILE | A | 469 | 35.956 | 39.801 | 83.112 | 1.00 | 26.94 |
|    | ATOM | 3725 | CG2 | ILE | A | 469 | 36.537 | 40.208 | 85.496 | 1.00 | 25.56 |
| 25 | ATOM | 3726 | CD1 | ILE | A | 469 | 36.247 | 38.298 | 83.085 | 1.00 | 45.50 |
|    | ATOM | 3727 | N   | ALA | A | 470 | 38.830 | 42.960 | 84.534 | 1.00 | 23.28 |
|    | ATOM | 3728 | CA  | ALA | A | 470 | 39.749 | 43.621 | 85.461 | 1.00 | 22.23 |
|    | ATOM | 3729 | C   | ALA | A | 470 | 39.392 | 45.038 | 85.808 | 1.00 | 30.29 |
|    | ATOM | 3730 | O   | ALA | A | 470 | 39.474 | 45.451 | 86.986 | 1.00 | 32.82 |
| 30 | ATOM | 3731 | CB  | ALA | A | 470 | 41.218 | 43.502 | 85.074 | 1.00 | 21.98 |
|    | ATOM | 3732 | N   | LEU | A | 471 | 39.007 | 45.760 | 84.759 | 1.00 | 23.53 |
|    | ATOM | 3733 | CA  | LEU | A | 471 | 38.643 | 47.173 | 84.834 | 1.00 | 18.39 |
|    | ATOM | 3734 | C   | LEU | A | 471 | 37.333 | 47.373 | 85.569 | 1.00 | 26.57 |
|    | ATOM | 3735 | O   | LEU | A | 471 | 37.210 | 48.208 | 86.462 | 1.00 | 30.48 |
| 35 | ATOM | 3736 | CB  | LEU | A | 471 | 38.676 | 47.827 | 83.444 | 1.00 | 15.51 |
|    | ATOM | 3737 | CG  | LEU | A | 471 | 38.671 | 49.325 | 83.539 | 1.00 | 24.20 |
|    | ATOM | 3738 | CD1 | LEU | A | 471 | 39.754 | 49.795 | 84.513 | 1.00 | 24.86 |
|    | ATOM | 3739 | CD2 | LEU | A | 471 | 38.876 | 49.941 | 82.156 | 1.00 | 26.35 |
|    | ATOM | 3740 | N   | SER | A | 472 | 36.351 | 46.570 | 85.222 | 1.00 | 25.31 |
| 40 | ATOM | 3741 | CA  | SER | A | 472 | 35.080 | 46.674 | 85.901 | 1.00 | 27.56 |
|    | ATOM | 3742 | C   | SER | A | 472 | 35.260 | 46.477 | 87.396 | 1.00 | 33.46 |
|    | ATOM | 3743 | O   | SER | A | 472 | 34.800 | 47.292 | 88.214 | 1.00 | 32.85 |
|    | ATOM | 3744 | CB  | SER | A | 472 | 33.989 | 45.714 | 85.393 | 1.00 | 32.06 |
|    | ATOM | 3745 | OG  | SER | A | 472 | 34.492 | 44.774 | 84.470 | 1.00 | 48.56 |
| 45 | ATOM | 3746 | N   | GLN | A | 473 | 35.911 | 45.350 | 87.736 | 1.00 | 27.52 |
|    | ATOM | 3747 | CA  | GLN | A | 473 | 36.170 | 44.971 | 89.108 | 1.00 | 24.10 |
|    | ATOM | 3748 | C   | GLN | A | 473 | 36.866 | 46.096 | 89.836 | 1.00 | 25.18 |
|    | ATOM | 3749 | O   | GLN | A | 473 | 36.534 | 46.458 | 90.969 | 1.00 | 21.62 |
|    | ATOM | 3750 | CB  | GLN | A | 473 | 36.994 | 43.671 | 89.148 | 1.00 | 25.86 |
| 50 | ATOM | 3751 | CG  | GLN | A | 473 | 36.128 | 42.402 | 89.118 | 1.00 | 32.72 |
|    | ATOM | 3752 | CD  | GLN | A | 473 | 34.970 | 42.504 | 90.090 | 1.00 | 46.08 |
|    | ATOM | 3753 | OE1 | GLN | A | 473 | 35.165 | 42.422 | 91.308 | 1.00 | 40.73 |
|    | ATOM | 3754 | NE2 | GLN | A | 473 | 33.761 | 42.692 | 89.559 | 1.00 | 28.28 |
|    | ATOM | 3755 | N   | ARG | A | 474 | 37.855 | 46.656 | 89.161 | 1.00 | 24.00 |
| 55 | ATOM | 3756 | CA  | ARG | A | 474 | 38.562 | 47.765 | 89.779 | 1.00 | 24.46 |
|    | ATOM | 3757 | C   | ARG | A | 474 | 37.609 | 48.893 | 90.141 | 1.00 | 29.31 |
|    | ATOM | 3758 | O   | ARG | A | 474 | 37.620 | 49.447 | 91.242 | 1.00 | 33.13 |
|    | ATOM | 3759 | CB  | ARG | A | 474 | 39.682 | 48.290 | 88.898 | 1.00 | 20.19 |
|    | ATOM | 3760 | CG  | ARG | A | 474 | 40.866 | 47.352 | 88.831 | 1.00 | 28.48 |
| 60 | ATOM | 3761 | CD  | ARG | A | 474 | 41.871 | 47.869 | 87.832 | 1.00 | 34.41 |
|    | ATOM | 3762 | NE  | ARG | A | 474 | 42.258 | 49.245 | 88.093 | 1.00 | 40.09 |
|    | ATOM | 3763 | CZ  | ARG | A | 474 | 42.927 | 49.938 | 87.185 | 1.00 | 51.25 |
|    | ATOM | 3764 | NH1 | ARG | A | 474 | 43.220 | 49.376 | 86.019 | 1.00 | 24.79 |
|    | ATOM | 3765 | NH2 | ARG | A | 474 | 43.316 | 51.199 | 87.444 | 1.00 | 20.43 |
|    | ATOM | 3766 | N   | TRP | A | 475 | 36.791 | 49.259 | 89.178 | 1.00 | 25.32 |



|    |      |      |     |     |   |     |        |        |         |      |        |
|----|------|------|-----|-----|---|-----|--------|--------|---------|------|--------|
|    | ATOM | 3767 | CA  | TRP | A | 475 | 35.862 | 50.332 | 89.400  | 1.00 | 26.77  |
|    | ATOM | 3768 | C   | TRP | A | 475 | 34.881 | 49.962 | 90.474  | 1.00 | 27.52  |
|    | ATOM | 3769 | O   | TRP | A | 475 | 34.749 | 50.633 | 91.475  | 1.00 | 29.64  |
| 5  | ATOM | 3770 | CB  | TRP | A | 475 | 35.199 | 50.804 | 88.093  | 1.00 | 27.95  |
|    | ATOM | 3771 | CG  | TRP | A | 475 | 36.047 | 51.819 | 87.361  | 1.00 | 32.11  |
|    | ATOM | 3772 | CD1 | TRP | A | 475 | 36.873 | 51.592 | 86.298  | 1.00 | 35.65  |
|    | ATOM | 3773 | CD2 | TRP | A | 475 | 36.161 | 53.217 | 87.648  | 1.00 | 31.62  |
|    | ATOM | 3774 | NE1 | TRP | A | 475 | 37.484 | 52.748 | 85.904  | 1.00 | 34.92  |
|    | ATOM | 3775 | CE2 | TRP | A | 475 | 37.054 | 53.763 | 86.707  | 1.00 | 36.16  |
| 10 | ATOM | 3776 | CE3 | TRP | A | 475 | 35.588 | 54.040 | 88.606  | 1.00 | 32.63  |
|    | ATOM | 3777 | CZ2 | TRP | A | 475 | 37.372 | 55.112 | 86.719  | 1.00 | 36.24  |
|    | ATOM | 3778 | CZ3 | TRP | A | 475 | 35.897 | 55.375 | 88.616  | 1.00 | 34.74  |
|    | ATOM | 3779 | CH2 | TRP | A | 475 | 36.777 | 55.901 | 87.685  | 1.00 | 35.77  |
|    | ATOM | 3780 | N   | ILE | A | 476 | 34.234 | 48.847 | 90.279  | 1.00 | 26.36  |
| 15 | ATOM | 3781 | CA  | ILE | A | 476 | 33.268 | 48.386 | 91.235  | 1.00 | 28.33  |
|    | ATOM | 3782 | C   | ILE | A | 476 | 33.771 | 48.315 | 92.681  | 1.00 | 34.20  |
|    | ATOM | 3783 | O   | ILE | A | 476 | 33.056 | 48.595 | 93.637  | 1.00 | 36.89  |
|    | ATOM | 3784 | CB  | ILE | A | 476 | 32.722 | 47.070 | 90.761  | 1.00 | 32.23  |
|    | ATOM | 3785 | CG1 | ILE | A | 476 | 31.993 | 47.308 | 89.443  | 1.00 | 30.49  |
| 20 | ATOM | 3786 | CG2 | ILE | A | 476 | 31.864 | 46.376 | 91.851  | 1.00 | 34.86  |
|    | ATOM | 3787 | CD1 | ILE | A | 476 | 31.595 | 46.005 | 88.756  | 1.00 | 33.04  |
|    | ATOM | 3788 | N   | THR | A | 477 | 35.010 | 47.934 | 92.860  | 1.00 | 27.27  |
|    | ATOM | 3789 | CA  | THR | A | 477 | 35.558 | 47.846 | 94.194  | 1.00 | 24.15  |
|    | ATOM | 3790 | C   | THR | A | 477 | 36.416 | 49.052 | 94.523  | 1.00 | 27.30  |
| 25 | ATOM | 3791 | O   | THR | A | 477 | 37.120 | 49.065 | 95.519  | 1.00 | 27.36  |
|    | ATOM | 3792 | CB  | THR | A | 477 | 36.402 | 46.578 | 94.257  | 1.00 | 32.13  |
|    | ATOM | 3793 | OG1 | THR | A | 477 | 37.593 | 46.848 | 93.557  | 1.00 | 29.48  |
|    | ATOM | 3794 | CG2 | THR | A | 477 | 35.634 | 45.470 | 93.530  | 1.00 | 16.94  |
|    | ATOM | 3795 | N   | ALA | A | 478 | 36.371 | 50.097 | 93.695  | 1.00 | 22.33  |
| 30 | ATOM | 3796 | CA  | ALA | A | 478 | 37.164 | 51.260 | 93.988  | 1.00 | 20.44  |
|    | ATOM | 3797 | C   | ALA | A | 478 | 36.890 | 51.843 | 95.390  | 1.00 | 32.94  |
|    | ATOM | 3798 | O   | ALA | A | 478 | 35.786 | 51.756 | 95.922  | 1.00 | 34.38  |
|    | ATOM | 3799 | CB  | ALA | A | 478 | 36.938 | 52.343 | 92.942  | 1.00 | 19.26  |
|    | ATOM | 3800 | N   | LYS | A | 479 | 37.931 | 52.469 | 95.970  | 1.00 | 29.65  |
| 35 | ATOM | 3801 | CA  | LYS | A | 479 | 37.899 | 53.168 | 97.243  | 1.00 | 27.30  |
|    | ATOM | 3802 | C   | LYS | A | 479 | 38.575 | 54.512 | 97.051  | 1.00 | 36.54  |
|    | ATOM | 3803 | O   | LYS | A | 479 | 39.378 | 54.692 | 96.118  | 1.00 | 34.13  |
|    | ATOM | 3804 | CB  | LYS | A | 479 | 38.457 | 52.410 | 98.417  | 1.00 | 28.01  |
|    | ATOM | 3805 | CG  | LYS | A | 479 | 37.696 | 51.116 | 98.631  | 1.00 | 51.38  |
| 40 | ATOM | 3806 | CD  | LYS | A | 479 | 37.115 | 50.880 | 100.021 | 1.00 | 67.24  |
|    | ATOM | 3807 | CE  | LYS | A | 479 | 35.804 | 50.103 | 99.931  | 1.00 | 87.12  |
|    | ATOM | 3808 | NZ  | LYS | A | 479 | 35.711 | 48.948 | 100.841 | 1.00 | 85.55  |
|    | ATOM | 3809 | N   | GLU | A | 480 | 38.241 | 55.477 | 97.900  | 1.00 | 36.30  |
| 45 | ATOM | 3810 | CA  | GLU | A | 480 | 38.843 | 56.793 | 97.751  | 1.00 | 34.79  |
|    | ATOM | 3811 | C   | GLU | A | 480 | 40.261 | 56.707 | 97.220  | 1.00 | 34.79  |
|    | ATOM | 3812 | O   | GLU | A | 480 | 40.613 | 57.332 | 96.234  | 1.00 | 34.10  |
|    | ATOM | 3813 | CB  | GLU | A | 480 | 38.899 | 57.565 | 99.078  | 1.00 | 36.21  |
|    | ATOM | 3814 | CG  | GLU | A | 480 | 37.709 | 58.500 | 99.303  | 1.00 | 63.85  |
|    | ATOM | 3815 | CD  | GLU | A | 480 | 37.601 | 59.511 | 98.214  | 1.00 | 100.00 |
| 50 | ATOM | 3816 | OE1 | GLU | A | 480 | 38.457 | 59.648 | 97.357  | 1.00 | 100.00 |
|    | ATOM | 3817 | OE2 | GLU | A | 480 | 36.491 | 60.209 | 98.288  | 1.00 | 100.00 |
|    | ATOM | 3818 | N   | ASP | A | 481 | 41.080 | 55.946 | 97.904  | 1.00 | 24.69  |
|    | ATOM | 3819 | CA  | ASP | A | 481 | 42.451 | 55.860 | 97.519  | 1.00 | 23.87  |
|    | ATOM | 3820 | C   | ASP | A | 481 | 42.771 | 55.314 | 96.132  | 1.00 | 34.51  |
| 55 | ATOM | 3821 | O   | ASP | A | 481 | 43.925 | 55.312 | 95.721  | 1.00 | 39.44  |
|    | ATOM | 3822 | CB  | ASP | A | 481 | 43.262 | 55.155 | 98.611  | 1.00 | 25.29  |
|    | ATOM | 3823 | CG  | ASP | A | 481 | 43.072 | 53.668 | 98.575  | 1.00 | 39.58  |
|    | ATOM | 3824 | OD1 | ASP | A | 481 | 42.471 | 53.029 | 97.708  | 1.00 | 46.00  |
|    | ATOM | 3825 | OD2 | ASP | A | 481 | 43.698 | 53.107 | 99.567  | 1.00 | 39.59  |
| 60 | ATOM | 3826 | N   | ASP | A | 482 | 41.788 | 54.881 | 95.373  | 1.00 | 30.70  |
|    | ATOM | 3827 | CA  | ASP | A | 482 | 42.098 | 54.379 | 94.024  | 1.00 | 31.73  |
|    | ATOM | 3828 | C   | ASP | A | 482 | 41.725 | 55.307 | 92.859  | 1.00 | 34.17  |
|    | ATOM | 3829 | O   | ASP | A | 482 | 42.158 | 55.150 | 91.717  | 1.00 | 35.45  |
|    | ATOM | 3830 | CB  | ASP | A | 482 | 41.399 | 53.022 | 93.756  | 1.00 | 33.31  |



|    |      |      |     |     |   |     |        |        |        |      |        |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
|    | ATOM | 3831 | CG  | ASP | A | 482 | 41.686 | 51.970 | 94.779 | 1.00 | 38.90  |
|    | ATOM | 3832 | OD1 | ASP | A | 482 | 42.810 | 51.514 | 94.992 | 1.00 | 42.45  |
|    | ATOM | 3833 | OD2 | ASP | A | 482 | 40.606 | 51.625 | 95.440 | 1.00 | 40.17  |
| 5  | ATOM | 3834 | N   | LEU | A | 483 | 40.863 | 56.246 | 93.146 | 1.00 | 29.93  |
|    | ATOM | 3835 | CA  | LEU | A | 483 | 40.352 | 57.159 | 92.160 | 1.00 | 27.80  |
|    | ATOM | 3836 | C   | LEU | A | 483 | 41.434 | 57.943 | 91.410 | 1.00 | 40.70  |
|    | ATOM | 3837 | O   | LEU | A | 483 | 41.386 | 58.102 | 90.180 | 1.00 | 40.76  |
|    | ATOM | 3838 | CB  | LEU | A | 483 | 39.265 | 58.049 | 92.819 | 1.00 | 22.54  |
| 10 | ATOM | 3839 | CG  | LEU | A | 483 | 38.148 | 57.240 | 93.488 | 1.00 | 20.75  |
|    | ATOM | 3840 | CD1 | LEU | A | 483 | 37.170 | 58.165 | 94.197 | 1.00 | 19.29  |
|    | ATOM | 3841 | CD2 | LEU | A | 483 | 37.389 | 56.467 | 92.414 | 1.00 | 21.46  |
|    | ATOM | 3842 | N   | ASN | A | 484 | 42.410 | 58.446 | 92.162 | 1.00 | 36.15  |
|    | ATOM | 3843 | CA  | ASN | A | 484 | 43.459 | 59.225 | 91.571 | 1.00 | 34.08  |
| 15 | ATOM | 3844 | C   | ASN | A | 484 | 44.168 | 58.524 | 90.429 | 1.00 | 39.51  |
|    | ATOM | 3845 | O   | ASN | A | 484 | 44.456 | 59.091 | 89.359 | 1.00 | 38.59  |
|    | ATOM | 3846 | CB  | ASN | A | 484 | 44.495 | 59.602 | 92.618 | 1.00 | 34.26  |
|    | ATOM | 3847 | CG  | ASN | A | 484 | 45.807 | 59.955 | 91.941 | 1.00 | 100.00 |
|    | ATOM | 3848 | OD1 | ASN | A | 484 | 45.878 | 60.940 | 91.171 | 1.00 | 100.00 |
| 20 | ATOM | 3849 | ND2 | ASN | A | 484 | 46.836 | 59.134 | 92.186 | 1.00 | 100.00 |
|    | ATOM | 3850 | N   | SER | A | 485 | 44.472 | 57.268 | 90.698 | 1.00 | 35.37  |
|    | ATOM | 3851 | CA  | SER | A | 485 | 45.202 | 56.417 | 89.791 | 1.00 | 32.79  |
|    | ATOM | 3852 | C   | SER | A | 485 | 44.522 | 56.140 | 88.484 | 1.00 | 32.26  |
|    | ATOM | 3853 | O   | SER | A | 485 | 45.159 | 55.925 | 87.463 | 1.00 | 32.44  |
| 25 | ATOM | 3854 | CB  | SER | A | 485 | 45.565 | 55.132 | 90.477 | 1.00 | 38.65  |
|    | ATOM | 3855 | OG  | SER | A | 485 | 46.040 | 55.437 | 91.777 | 1.00 | 62.66  |
|    | ATOM | 3856 | N   | PHE | A | 486 | 43.222 | 56.110 | 88.491 | 1.00 | 27.13  |
|    | ATOM | 3857 | CA  | PHE | A | 486 | 42.631 | 55.809 | 87.233 | 1.00 | 28.26  |
|    | ATOM | 3858 | C   | PHE | A | 486 | 43.193 | 56.772 | 86.264 | 1.00 | 32.12  |
| 30 | ATOM | 3859 | O   | PHE | A | 486 | 43.423 | 57.910 | 86.604 | 1.00 | 32.02  |
|    | ATOM | 3860 | CB  | PHE | A | 486 | 41.101 | 55.819 | 87.198 | 1.00 | 31.01  |
|    | ATOM | 3861 | CG  | PHE | A | 486 | 40.471 | 54.807 | 88.132 | 1.00 | 27.04  |
|    | ATOM | 3862 | CD1 | PHE | A | 486 | 40.504 | 53.425 | 87.911 | 1.00 | 22.43  |
|    | ATOM | 3863 | CD2 | PHE | A | 486 | 39.805 | 55.293 | 89.253 | 1.00 | 21.40  |
| 35 | ATOM | 3864 | CE1 | PHE | A | 486 | 39.896 | 52.538 | 88.804 | 1.00 | 19.69  |
|    | ATOM | 3865 | CE2 | PHE | A | 486 | 39.224 | 54.426 | 90.174 | 1.00 | 19.20  |
|    | ATOM | 3866 | CZ  | PHE | A | 486 | 39.245 | 53.051 | 89.927 | 1.00 | 15.13  |
|    | ATOM | 3867 | N   | ASN | A | 487 | 43.455 | 56.279 | 85.089 | 1.00 | 34.97  |
|    | ATOM | 3868 | CA  | ASN | A | 487 | 44.032 | 57.092 | 84.070 | 1.00 | 38.06  |
| 40 | ATOM | 3869 | C   | ASN | A | 487 | 43.491 | 56.622 | 82.758 | 1.00 | 43.55  |
|    | ATOM | 3870 | O   | ASN | A | 487 | 42.951 | 55.537 | 82.604 | 1.00 | 46.30  |
|    | ATOM | 3871 | CB  | ASN | A | 487 | 45.591 | 57.038 | 84.085 | 1.00 | 43.93  |
|    | ATOM | 3872 | CG  | ASN | A | 487 | 46.196 | 58.169 | 83.302 | 1.00 | 56.10  |
|    | ATOM | 3873 | OD1 | ASN | A | 487 | 46.057 | 58.189 | 82.077 | 1.00 | 42.12  |
| 45 | ATOM | 3874 | ND2 | ASN | A | 487 | 46.829 | 59.112 | 84.007 | 1.00 | 65.62  |
|    | ATOM | 3875 | N   | ALA | A | 488 | 43.662 | 57.435 | 81.781 | 1.00 | 39.34  |
|    | ATOM | 3876 | CA  | ALA | A | 488 | 43.201 | 57.055 | 80.472 | 1.00 | 38.25  |
|    | ATOM | 3877 | C   | ALA | A | 488 | 44.024 | 55.900 | 79.809 | 1.00 | 43.58  |
|    | ATOM | 3878 | O   | ALA | A | 488 | 43.596 | 55.317 | 78.834 | 1.00 | 44.11  |
| 50 | ATOM | 3879 | CB  | ALA | A | 488 | 43.153 | 58.314 | 79.621 | 1.00 | 37.54  |
|    | ATOM | 3880 | N   | THR | A | 489 | 45.207 | 55.555 | 80.314 | 1.00 | 38.34  |
|    | ATOM | 3881 | CA  | THR | A | 489 | 45.996 | 54.499 | 79.715 | 1.00 | 36.16  |
|    | ATOM | 3882 | C   | THR | A | 489 | 45.270 | 53.181 | 79.792 | 1.00 | 45.74  |
|    | ATOM | 3883 | O   | THR | A | 489 | 45.476 | 52.233 | 79.057 | 1.00 | 47.78  |
| 55 | ATOM | 3884 | CB  | THR | A | 489 | 47.296 | 54.458 | 80.503 | 1.00 | 31.01  |
|    | ATOM | 3885 | OG1 | THR | A | 489 | 46.961 | 54.457 | 81.872 | 1.00 | 35.33  |
|    | ATOM | 3886 | CG2 | THR | A | 489 | 47.993 | 55.771 | 80.229 | 1.00 | 28.28  |
|    | ATOM | 3887 | N   | ASP | A | 490 | 44.337 | 53.182 | 80.708 | 1.00 | 46.75  |
|    | ATOM | 3888 | CA  | ASP | A | 490 | 43.560 | 52.018 | 80.972 | 1.00 | 51.49  |
| 60 | ATOM | 3889 | C   | ASP | A | 490 | 42.759 | 51.515 | 79.786 | 1.00 | 52.21  |
|    | ATOM | 3890 | O   | ASP | A | 490 | 42.396 | 50.342 | 79.651 | 1.00 | 54.75  |
|    | ATOM | 3891 | CB  | ASP | A | 490 | 42.676 | 52.345 | 82.184 | 1.00 | 54.04  |
|    | ATOM | 3892 | CG  | ASP | A | 490 | 43.413 | 52.884 | 83.380 | 1.00 | 53.83  |
|    | ATOM | 3893 | OD1 | ASP | A | 490 | 44.621 | 52.777 | 83.616 | 1.00 | 62.93  |
|    | ATOM | 3894 | OD2 | ASP | A | 490 | 42.565 | 53.446 | 84.165 | 1.00 | 35.66  |



|    |      |      |     |     |   |     |        |        |        |      |        |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
|    | ATOM | 3895 | N   | LEU | A | 491 | 42.486 | 52.450 | 78.938 | 1.00 | 42.42  |
|    | ATOM | 3896 | CA  | LEU | A | 491 | 41.752 | 52.250 | 77.723 | 1.00 | 43.54  |
|    | ATOM | 3897 | C   | LEU | A | 491 | 42.712 | 51.977 | 76.585 | 1.00 | 43.97  |
| 5  | ATOM | 3898 | O   | LEU | A | 491 | 42.340 | 51.438 | 75.588 | 1.00 | 42.53  |
|    | ATOM | 3899 | CB  | LEU | A | 491 | 40.984 | 53.528 | 77.421 | 1.00 | 44.89  |
|    | ATOM | 3900 | CG  | LEU | A | 491 | 39.794 | 53.747 | 78.338 | 1.00 | 48.31  |
|    | ATOM | 3901 | CD1 | LEU | A | 491 | 38.558 | 54.171 | 77.552 | 1.00 | 49.16  |
|    | ATOM | 3902 | CD2 | LEU | A | 491 | 39.377 | 52.494 | 79.125 | 1.00 | 39.24  |
| 10 | ATOM | 3903 | N   | LYS | A | 492 | 43.958 | 52.403 | 76.754 | 1.00 | 42.32  |
|    | ATOM | 3904 | CA  | LYS | A | 492 | 44.999 | 52.320 | 75.696 | 1.00 | 44.57  |
|    | ATOM | 3905 | C   | LYS | A | 492 | 44.826 | 51.165 | 74.680 | 1.00 | 49.08  |
|    | ATOM | 3906 | O   | LYS | A | 492 | 44.810 | 51.343 | 73.473 | 1.00 | 49.66  |
|    | ATOM | 3907 | CB  | LYS | A | 492 | 46.359 | 52.177 | 76.401 | 1.00 | 48.47  |
| 15 | ATOM | 3908 | CG  | LYS | A | 492 | 47.487 | 52.883 | 75.629 | 1.00 | 88.73  |
|    | ATOM | 3909 | CD  | LYS | A | 492 | 48.852 | 52.537 | 76.197 | 1.00 | 100.00 |
|    | ATOM | 3910 | CE  | LYS | A | 492 | 48.786 | 51.460 | 77.300 | 1.00 | 100.00 |
|    | ATOM | 3911 | NZ  | LYS | A | 492 | 50.103 | 50.896 | 77.541 | 1.00 | 100.00 |
|    | ATOM | 3912 | N   | ASP | A | 493 | 44.711 | 49.917 | 75.227 | 1.00 | 41.86  |
| 20 | ATOM | 3913 | CA  | ASP | A | 493 | 44.664 | 48.740 | 74.372 | 1.00 | 40.17  |
|    | ATOM | 3914 | C   | ASP | A | 493 | 43.220 | 48.162 | 74.215 | 1.00 | 44.29  |
|    | ATOM | 3915 | O   | ASP | A | 493 | 43.031 | 46.973 | 73.889 | 1.00 | 42.00  |
|    | ATOM | 3916 | CB  | ASP | A | 493 | 45.560 | 47.699 | 75.015 | 1.00 | 41.52  |
|    | ATOM | 3917 | CG  | ASP | A | 493 | 47.021 | 48.130 | 74.956 | 1.00 | 67.01  |
| 25 | ATOM | 3918 | OD1 | ASP | A | 493 | 47.467 | 48.451 | 73.856 | 1.00 | 77.10  |
|    | ATOM | 3919 | OD2 | ASP | A | 493 | 47.678 | 48.131 | 75.984 | 1.00 | 57.19  |
|    | ATOM | 3920 | N   | LEU | A | 494 | 42.193 | 49.005 | 74.475 | 1.00 | 40.69  |
|    | ATOM | 3921 | CA  | LEU | A | 494 | 40.789 | 48.512 | 74.526 | 1.00 | 36.32  |
|    | ATOM | 3922 | C   | LEU | A | 494 | 39.992 | 48.877 | 73.245 | 1.00 | 37.76  |
| 30 | ATOM | 3923 | O   | LEU | A | 494 | 39.897 | 50.029 | 72.863 | 1.00 | 38.93  |
|    | ATOM | 3924 | CB  | LEU | A | 494 | 40.098 | 49.125 | 75.733 | 1.00 | 32.52  |
|    | ATOM | 3925 | CG  | LEU | A | 494 | 40.376 | 48.433 | 77.063 | 1.00 | 30.66  |
|    | ATOM | 3926 | CD1 | LEU | A | 494 | 39.229 | 48.580 | 78.052 | 1.00 | 30.39  |
|    | ATOM | 3927 | CD2 | LEU | A | 494 | 40.611 | 46.925 | 76.918 | 1.00 | 23.54  |
| 35 | ATOM | 3928 | N   | SER | A | 495 | 39.477 | 47.825 | 72.631 | 1.00 | 25.56  |
|    | ATOM | 3929 | CA  | SER | A | 495 | 38.674 | 48.017 | 71.457 | 1.00 | 22.23  |
|    | ATOM | 3930 | C   | SER | A | 495 | 37.344 | 48.670 | 71.856 | 1.00 | 31.27  |
|    | ATOM | 3931 | O   | SER | A | 495 | 36.968 | 48.706 | 73.038 | 1.00 | 31.21  |
|    | ATOM | 3932 | CB  | SER | A | 495 | 38.380 | 46.705 | 70.795 | 1.00 | 20.88  |
| 40 | ATOM | 3933 | OG  | SER | A | 495 | 37.192 | 46.143 | 71.317 | 1.00 | 33.60  |
|    | ATOM | 3934 | N   | SER | A | 496 | 36.627 | 49.184 | 70.865 | 1.00 | 29.48  |
|    | ATOM | 3935 | CA  | SER | A | 496 | 35.363 | 49.821 | 71.139 | 1.00 | 26.67  |
|    | ATOM | 3936 | C   | SER | A | 496 | 34.495 | 48.747 | 71.744 | 1.00 | 29.54  |
|    | ATOM | 3937 | O   | SER | A | 496 | 33.744 | 48.960 | 72.697 | 1.00 | 24.80  |
| 45 | ATOM | 3938 | CB  | SER | A | 496 | 34.760 | 50.441 | 69.894 | 1.00 | 24.67  |
|    | ATOM | 3939 | OG  | SER | A | 496 | 33.749 | 49.597 | 69.397 | 1.00 | 48.80  |
|    | ATOM | 3940 | N   | HIS | A | 497 | 34.674 | 47.547 | 71.219 | 1.00 | 26.61  |
|    | ATOM | 3941 | CA  | HIS | A | 497 | 33.949 | 46.383 | 71.750 | 1.00 | 29.22  |
|    | ATOM | 3942 | C   | HIS | A | 497 | 34.156 | 46.148 | 73.275 | 1.00 | 37.24  |
| 50 | ATOM | 3943 | O   | HIS | A | 497 | 33.238 | 45.863 | 74.041 | 1.00 | 38.21  |
|    | ATOM | 3944 | CB  | HIS | A | 497 | 34.364 | 45.106 | 70.978 | 1.00 | 30.69  |
|    | ATOM | 3945 | CG  | HIS | A | 497 | 34.182 | 45.348 | 69.545 | 1.00 | 34.29  |
|    | ATOM | 3946 | ND1 | HIS | A | 497 | 32.943 | 45.204 | 68.962 | 1.00 | 35.42  |
|    | ATOM | 3947 | CD2 | HIS | A | 497 | 35.054 | 45.833 | 68.622 | 1.00 | 36.68  |
| 55 | ATOM | 3948 | CE1 | HIS | A | 497 | 33.075 | 45.531 | 67.702 | 1.00 | 35.05  |
|    | ATOM | 3949 | NE2 | HIS | A | 497 | 34.330 | 45.932 | 67.462 | 1.00 | 35.88  |
|    | ATOM | 3950 | N   | GLN | A | 498 | 35.406 | 46.243 | 73.715 | 1.00 | 33.56  |
|    | ATOM | 3951 | CA  | GLN | A | 498 | 35.737 | 46.008 | 75.094 | 1.00 | 29.69  |
|    | ATOM | 3952 | C   | GLN | A | 498 | 35.263 | 47.122 | 75.965 | 1.00 | 27.11  |
| 60 | ATOM | 3953 | O   | GLN | A | 498 | 34.842 | 46.930 | 77.089 | 1.00 | 23.92  |
|    | ATOM | 3954 | CB  | GLN | A | 498 | 37.221 | 45.659 | 75.248 | 1.00 | 29.95  |
|    | ATOM | 3955 | CG  | GLN | A | 498 | 37.582 | 44.317 | 74.544 | 1.00 | 25.78  |
|    | ATOM | 3956 | CD  | GLN | A | 498 | 39.074 | 44.084 | 74.535 | 1.00 | 28.64  |
|    | ATOM | 3957 | OE1 | GLN | A | 498 | 39.796 | 44.891 | 73.960 | 1.00 | 26.62  |
|    | ATOM | 3958 | NE2 | GLN | A | 498 | 39.561 | 43.049 | 75.218 | 1.00 | 20.96  |



|    |      |      |     |           |        |        |        |      |       |
|----|------|------|-----|-----------|--------|--------|--------|------|-------|
|    | ATOM | 3959 | N   | LEU A 499 | 35.289 | 48.301 | 75.431 | 1.00 | 27.13 |
|    | ATOM | 3960 | CA  | LEU A 499 | 34.819 | 49.396 | 76.229 | 1.00 | 29.32 |
|    | ATOM | 3961 | C   | LEU A 499 | 33.351 | 49.162 | 76.632 | 1.00 | 28.39 |
| 5  | ATOM | 3962 | O   | LEU A 499 | 32.893 | 49.361 | 77.780 | 1.00 | 29.41 |
|    | ATOM | 3963 | CB  | LEU A 499 | 34.991 | 50.709 | 75.436 | 1.00 | 31.70 |
|    | ATOM | 3964 | CG  | LEU A 499 | 36.242 | 51.512 | 75.788 | 1.00 | 39.76 |
|    | ATOM | 3965 | CD1 | LEU A 499 | 37.335 | 50.572 | 76.278 | 1.00 | 42.91 |
|    | ATOM | 3966 | CD2 | LEU A 499 | 36.718 | 52.268 | 74.555 | 1.00 | 39.08 |
| 10 | ATOM | 3967 | N   | ASN A 500 | 32.606 | 48.737 | 75.642 | 1.00 | 15.23 |
|    | ATOM | 3968 | CA  | ASN A 500 | 31.213 | 48.508 | 75.828 | 1.00 | 13.44 |
|    | ATOM | 3969 | C   | ASN A 500 | 30.919 | 47.455 | 76.864 | 1.00 | 18.98 |
|    | ATOM | 3970 | O   | ASN A 500 | 29.997 | 47.602 | 77.705 | 1.00 | 19.01 |
|    | ATOM | 3971 | CB  | ASN A 500 | 30.604 | 48.129 | 74.476 | 1.00 | 12.21 |
|    | ATOM | 3972 | CG  | ASN A 500 | 29.093 | 48.214 | 74.426 | 1.00 | 37.49 |
| 15 | ATOM | 3973 | OD1 | ASN A 500 | 28.433 | 49.151 | 74.930 | 1.00 | 36.17 |
|    | ATOM | 3974 | ND2 | ASN A 500 | 28.542 | 47.218 | 73.787 | 1.00 | 18.34 |
|    | ATOM | 3975 | N   | GLU A 501 | 31.699 | 46.366 | 76.743 | 1.00 | 14.20 |
|    | ATOM | 3976 | CA  | GLU A 501 | 31.626 | 45.224 | 77.625 | 1.00 | 13.27 |
|    | ATOM | 3977 | C   | GLU A 501 | 31.948 | 45.676 | 79.063 | 1.00 | 21.59 |
| 20 | ATOM | 3978 | O   | GLU A 501 | 31.175 | 45.463 | 80.009 | 1.00 | 25.02 |
|    | ATOM | 3979 | CB  | GLU A 501 | 32.446 | 44.057 | 77.053 | 1.00 | 14.95 |
|    | ATOM | 3980 | CG  | GLU A 501 | 32.371 | 42.827 | 77.989 | 1.00 | 30.40 |
|    | ATOM | 3981 | CD  | GLU A 501 | 30.946 | 42.399 | 78.199 | 1.00 | 39.28 |
|    | ATOM | 3982 | OE1 | GLU A 501 | 30.050 | 42.672 | 77.413 | 1.00 | 76.70 |
| 25 | ATOM | 3983 | OE2 | GLU A 501 | 30.780 | 41.694 | 79.292 | 1.00 | 46.10 |
|    | ATOM | 3984 | N   | PHE A 502 | 33.059 | 46.400 | 79.226 | 1.00 | 18.07 |
|    | ATOM | 3985 | CA  | PHE A 502 | 33.395 | 46.952 | 80.530 | 1.00 | 21.54 |
|    | ATOM | 3986 | C   | PHE A 502 | 32.179 | 47.679 | 81.125 | 1.00 | 23.38 |
|    | ATOM | 3987 | O   | PHE A 502 | 31.786 | 47.491 | 82.301 | 1.00 | 21.47 |
| 30 | ATOM | 3988 | CB  | PHE A 502 | 34.507 | 48.012 | 80.327 | 1.00 | 26.05 |
|    | ATOM | 3989 | CG  | PHE A 502 | 34.590 | 49.082 | 81.393 | 1.00 | 30.41 |
|    | ATOM | 3990 | CD1 | PHE A 502 | 35.085 | 48.781 | 82.662 | 1.00 | 29.68 |
|    | ATOM | 3991 | CD2 | PHE A 502 | 34.211 | 50.402 | 81.132 | 1.00 | 39.16 |
|    | ATOM | 3992 | CE1 | PHE A 502 | 35.183 | 49.773 | 83.638 | 1.00 | 31.12 |
| 35 | ATOM | 3993 | CE2 | PHE A 502 | 34.305 | 51.414 | 82.096 | 1.00 | 40.46 |
|    | ATOM | 3994 | CZ  | PHE A 502 | 34.812 | 51.090 | 83.352 | 1.00 | 35.41 |
|    | ATOM | 3995 | N   | LEU A 503 | 31.613 | 48.557 | 80.288 | 1.00 | 18.39 |
|    | ATOM | 3996 | CA  | LEU A 503 | 30.487 | 49.343 | 80.692 | 1.00 | 22.78 |
|    | ATOM | 3997 | C   | LEU A 503 | 29.337 | 48.491 | 81.178 | 1.00 | 31.04 |
| 40 | ATOM | 3998 | O   | LEU A 503 | 28.768 | 48.784 | 82.243 | 1.00 | 29.23 |
|    | ATOM | 3999 | CB  | LEU A 503 | 30.002 | 50.325 | 79.619 | 1.00 | 24.68 |
|    | ATOM | 4000 | CG  | LEU A 503 | 30.888 | 51.571 | 79.465 | 1.00 | 27.47 |
|    | ATOM | 4001 | CD1 | LEU A 503 | 30.415 | 52.376 | 78.259 | 1.00 | 24.86 |
|    | ATOM | 4002 | CD2 | LEU A 503 | 30.860 | 52.420 | 80.733 | 1.00 | 20.54 |
| 45 | ATOM | 4003 | N   | ALA A 504 | 29.012 | 47.444 | 80.378 | 1.00 | 27.79 |
|    | ATOM | 4004 | CA  | ALA A 504 | 27.911 | 46.474 | 80.643 | 1.00 | 24.63 |
|    | ATOM | 4005 | C   | ALA A 504 | 28.140 | 45.752 | 81.939 | 1.00 | 27.71 |
|    | ATOM | 4006 | O   | ALA A 504 | 27.265 | 45.577 | 82.817 | 1.00 | 28.62 |
|    | ATOM | 4007 | CB  | ALA A 504 | 27.762 | 45.482 | 79.496 | 1.00 | 23.87 |
| 50 | ATOM | 4008 | N   | GLN A 505 | 29.382 | 45.344 | 82.066 | 1.00 | 22.16 |
|    | ATOM | 4009 | CA  | GLN A 505 | 29.738 | 44.710 | 83.299 | 1.00 | 21.02 |
|    | ATOM | 4010 | C   | GLN A 505 | 29.489 | 45.737 | 84.423 | 1.00 | 31.26 |
|    | ATOM | 4011 | O   | GLN A 505 | 28.787 | 45.507 | 85.413 | 1.00 | 32.31 |
|    | ATOM | 4012 | CB  | GLN A 505 | 31.202 | 44.209 | 83.270 | 1.00 | 18.95 |
| 55 | ATOM | 4013 | CG  | GLN A 505 | 31.367 | 42.881 | 82.495 | 1.00 | 13.72 |
|    | ATOM | 4014 | CD  | GLN A 505 | 32.806 | 42.549 | 82.136 | 1.00 | 31.75 |
|    | ATOM | 4015 | OE1 | GLN A 505 | 33.796 | 42.969 | 82.768 | 1.00 | 43.14 |
|    | ATOM | 4016 | NE2 | GLN A 505 | 32.923 | 41.781 | 81.085 | 1.00 | 39.34 |
|    | ATOM | 4017 | N   | THR A 506 | 30.056 | 46.918 | 84.263 | 1.00 | 25.95 |
| 60 | ATOM | 4018 | CA  | THR A 506 | 29.855 | 47.864 | 85.302 | 1.00 | 23.64 |
|    | ATOM | 4019 | C   | THR A 506 | 28.411 | 48.101 | 85.579 | 1.00 | 23.89 |
|    | ATOM | 4020 | O   | THR A 506 | 27.923 | 47.999 | 86.696 | 1.00 | 22.75 |
|    | ATOM | 4021 | CB  | THR A 506 | 30.600 | 49.130 | 85.008 | 1.00 | 23.72 |
|    | ATOM | 4022 | OG1 | THR A 506 | 31.938 | 48.749 | 84.742 | 1.00 | 27.18 |



|    |      |      |     |     |   |     |        |        |        |      |        |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
|    | ATOM | 4023 | CG2 | THR | A | 506 | 30.502 | 49.961 | 86.260 | 1.00 | 11.12  |
|    | ATOM | 4024 | N   | LEU | A | 507 | 27.727 | 48.408 | 84.518 | 1.00 | 17.92  |
|    | ATOM | 4025 | CA  | LEU | A | 507 | 26.334 | 48.683 | 84.604 | 1.00 | 17.22  |
| 5  | ATOM | 4026 | C   | LEU | A | 507 | 25.618 | 47.683 | 85.442 | 1.00 | 25.65  |
|    | ATOM | 4027 | O   | LEU | A | 507 | 24.816 | 48.073 | 86.266 | 1.00 | 27.85  |
|    | ATOM | 4028 | CB  | LEU | A | 507 | 25.693 | 48.686 | 83.224 | 1.00 | 17.85  |
|    | ATOM | 4029 | CG  | LEU | A | 507 | 24.207 | 48.930 | 83.336 | 1.00 | 21.02  |
|    | ATOM | 4030 | CD1 | LEU | A | 507 | 23.974 | 50.290 | 83.970 | 1.00 | 22.48  |
| 10 | ATOM | 4031 | CD2 | LEU | A | 507 | 23.599 | 48.919 | 81.949 | 1.00 | 15.25  |
|    | ATOM | 4032 | N   | GLN | A | 508 | 25.878 | 46.395 | 85.194 | 1.00 | 21.35  |
|    | ATOM | 4033 | CA  | GLN | A | 508 | 25.215 | 45.333 | 85.979 | 1.00 | 18.08  |
|    | ATOM | 4034 | C   | GLN | A | 508 | 25.386 | 45.561 | 87.508 | 1.00 | 34.24  |
|    | ATOM | 4035 | O   | GLN | A | 508 | 24.653 | 45.017 | 88.343 | 1.00 | 34.04  |
| 15 | ATOM | 4036 | CB  | GLN | A | 508 | 25.713 | 43.917 | 85.608 | 1.00 | 10.94  |
|    | ATOM | 4037 | CG  | GLN | A | 508 | 25.366 | 43.446 | 84.191 | 1.00 | 26.42  |
|    | ATOM | 4038 | CD  | GLN | A | 508 | 25.635 | 41.944 | 84.002 | 1.00 | 52.93  |
|    | ATOM | 4039 | OE1 | GLN | A | 508 | 26.550 | 41.396 | 84.628 | 1.00 | 32.89  |
|    | ATOM | 4040 | NE2 | GLN | A | 508 | 24.864 | 41.252 | 83.147 | 1.00 | 34.36  |
| 20 | ATOM | 4041 | N   | ARG | A | 509 | 26.380 | 46.361 | 87.901 | 1.00 | 33.73  |
|    | ATOM | 4042 | CA  | ARG | A | 509 | 26.600 | 46.614 | 89.328 | 1.00 | 32.53  |
|    | ATOM | 4043 | C   | ARG | A | 509 | 26.153 | 48.016 | 89.727 | 1.00 | 33.63  |
|    | ATOM | 4044 | O   | ARG | A | 509 | 26.509 | 48.522 | 90.777 | 1.00 | 31.08  |
|    | ATOM | 4045 | CB  | ARG | A | 509 | 28.055 | 46.440 | 89.760 | 1.00 | 29.22  |
| 25 | ATOM | 4046 | CG  | ARG | A | 509 | 28.553 | 45.014 | 89.733 | 1.00 | 29.78  |
|    | ATOM | 4047 | CD  | ARG | A | 509 | 27.744 | 44.054 | 90.609 | 1.00 | 30.86  |
|    | ATOM | 4048 | NE  | ARG | A | 509 | 28.533 | 43.602 | 91.756 | 1.00 | 82.23  |
|    | ATOM | 4049 | CZ  | ARG | A | 509 | 29.842 | 43.274 | 91.726 | 1.00 | 100.00 |
|    | ATOM | 4050 | NH1 | ARG | A | 509 | 30.579 | 43.315 | 90.613 | 1.00 | 92.85  |
| 30 | ATOM | 4051 | NH2 | ARG | A | 509 | 30.430 | 42.881 | 92.855 | 1.00 | 91.85  |
|    | ATOM | 4052 | N   | ALA | A | 510 | 25.384 | 48.659 | 88.880 | 1.00 | 32.59  |
|    | ATOM | 4053 | CA  | ALA | A | 510 | 24.952 | 49.985 | 89.215 | 1.00 | 32.51  |
|    | ATOM | 4054 | C   | ALA | A | 510 | 24.151 | 49.845 | 90.479 | 1.00 | 34.97  |
|    | ATOM | 4055 | O   | ALA | A | 510 | 23.601 | 48.785 | 90.693 | 1.00 | 37.57  |
| 35 | ATOM | 4056 | CB  | ALA | A | 510 | 24.189 | 50.622 | 88.063 | 1.00 | 32.91  |
|    | ATOM | 4057 | N   | PRO | A | 511 | 24.174 | 50.856 | 91.334 | 1.00 | 25.14  |
|    | ATOM | 4058 | CA  | PRO | A | 511 | 24.867 | 52.102 | 91.052 | 1.00 | 21.00  |
|    | ATOM | 4059 | C   | PRO | A | 511 | 26.217 | 52.178 | 91.694 | 1.00 | 29.23  |
|    | ATOM | 4060 | O   | PRO | A | 511 | 26.445 | 51.601 | 92.723 | 1.00 | 28.16  |
| 40 | ATOM | 4061 | CB  | PRO | A | 511 | 24.102 | 53.169 | 91.818 | 1.00 | 21.55  |
|    | ATOM | 4062 | CG  | PRO | A | 511 | 23.316 | 52.432 | 92.886 | 1.00 | 28.68  |
|    | ATOM | 4063 | CD  | PRO | A | 511 | 23.169 | 50.995 | 92.407 | 1.00 | 25.16  |
|    | ATOM | 4064 | N   | LEU | A | 512 | 27.094 | 52.968 | 91.109 | 1.00 | 32.95  |
|    | ATOM | 4065 | CA  | LEU | A | 512 | 28.394 | 53.188 | 91.686 | 1.00 | 33.42  |
| 45 | ATOM | 4066 | C   | LEU | A | 512 | 28.287 | 54.512 | 92.397 | 1.00 | 38.65  |
|    | ATOM | 4067 | O   | LEU | A | 512 | 27.388 | 55.305 | 92.114 | 1.00 | 40.69  |
|    | ATOM | 4068 | CB  | LEU | A | 512 | 29.453 | 53.350 | 90.587 | 1.00 | 34.40  |
|    | ATOM | 4069 | CG  | LEU | A | 512 | 30.178 | 52.049 | 90.216 | 1.00 | 40.13  |
|    | ATOM | 4070 | CD1 | LEU | A | 512 | 29.222 | 51.086 | 89.508 | 1.00 | 39.04  |
| 50 | ATOM | 4071 | CD2 | LEU | A | 512 | 31.322 | 52.385 | 89.273 | 1.00 | 44.61  |
|    | ATOM | 4072 | N   | PRO | A | 513 | 29.196 | 54.781 | 93.312 | 1.00 | 31.05  |
|    | ATOM | 4073 | CA  | PRO | A | 513 | 29.167 | 56.058 | 94.008 | 1.00 | 27.16  |
|    | ATOM | 4074 | C   | PRO | A | 513 | 29.296 | 57.203 | 93.019 | 1.00 | 23.76  |
|    | ATOM | 4075 | O   | PRO | A | 513 | 30.121 | 57.182 | 92.118 | 1.00 | 27.17  |
| 55 | ATOM | 4076 | CB  | PRO | A | 513 | 30.387 | 56.013 | 94.948 | 1.00 | 25.59  |
|    | ATOM | 4077 | CG  | PRO | A | 513 | 30.702 | 54.542 | 95.149 | 1.00 | 27.14  |
|    | ATOM | 4078 | CD  | PRO | A | 513 | 30.030 | 53.779 | 94.032 | 1.00 | 25.00  |
|    | ATOM | 4079 | N   | LEU | A | 514 | 28.478 | 58.203 | 93.185 | 1.00 | 22.92  |
|    | ATOM | 4080 | CA  | LEU | A | 514 | 28.516 | 59.350 | 92.279 | 1.00 | 27.55  |
| 60 | ATOM | 4081 | C   | LEU | A | 514 | 29.930 | 59.766 | 91.940 | 1.00 | 31.95  |
|    | ATOM | 4082 | O   | LEU | A | 514 | 30.287 | 59.908 | 90.765 | 1.00 | 37.11  |
|    | ATOM | 4083 | CB  | LEU | A | 514 | 27.673 | 60.564 | 92.741 | 1.00 | 30.03  |
|    | ATOM | 4084 | CG  | LEU | A | 514 | 27.428 | 61.626 | 91.648 | 1.00 | 32.87  |
|    | ATOM | 4085 | CD1 | LEU | A | 514 | 26.648 | 61.082 | 90.440 | 1.00 | 28.48  |
|    | ATOM | 4086 | CD2 | LEU | A | 514 | 26.699 | 62.780 | 92.272 | 1.00 | 31.16  |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
|    | ATOM | 4087 | N   | GLY | A | 515 | 30.731 | 59.989 | 92.979 | 1.00 | 24.42 |
|    | ATOM | 4088 | CA  | GLY | A | 515 | 32.131 | 60.384 | 92.811 | 1.00 | 25.59 |
|    | ATOM | 4089 | C   | GLY | A | 515 | 32.902 | 59.472 | 91.835 | 1.00 | 33.83 |
|    | ATOM | 4090 | O   | GLY | A | 515 | 33.746 | 59.914 | 91.035 | 1.00 | 35.67 |
| 5  | ATOM | 4091 | N   | HIS | A | 516 | 32.602 | 58.180 | 91.891 | 1.00 | 26.40 |
|    | ATOM | 4092 | CA  | HIS | A | 516 | 33.257 | 57.255 | 90.998 | 1.00 | 25.86 |
|    | ATOM | 4093 | C   | HIS | A | 516 | 32.911 | 57.578 | 89.560 | 1.00 | 27.62 |
|    | ATOM | 4094 | O   | HIS | A | 516 | 33.786 | 57.596 | 88.695 | 1.00 | 28.67 |
| 10 | ATOM | 4095 | CB  | HIS | A | 516 | 32.826 | 55.814 | 91.282 | 1.00 | 25.39 |
|    | ATOM | 4096 | CG  | HIS | A | 516 | 33.452 | 55.283 | 92.505 | 1.00 | 27.96 |
|    | ATOM | 4097 | ND1 | HIS | A | 516 | 33.635 | 56.092 | 93.602 | 1.00 | 30.14 |
|    | ATOM | 4098 | CD2 | HIS | A | 516 | 33.929 | 54.037 | 92.791 | 1.00 | 27.79 |
|    | ATOM | 4099 | CE1 | HIS | A | 516 | 34.205 | 55.336 | 94.534 | 1.00 | 27.58 |
|    | ATOM | 4100 | NE2 | HIS | A | 516 | 34.390 | 54.099 | 94.085 | 1.00 | 27.02 |
| 15 | ATOM | 4101 | N   | ILE | A | 517 | 31.617 | 57.815 | 89.315 | 1.00 | 21.40 |
|    | ATOM | 4102 | CA  | ILE | A | 517 | 31.137 | 58.107 | 87.973 | 1.00 | 22.75 |
|    | ATOM | 4103 | C   | ILE | A | 517 | 31.706 | 59.424 | 87.462 | 1.00 | 31.09 |
|    | ATOM | 4104 | O   | ILE | A | 517 | 32.246 | 59.558 | 86.352 | 1.00 | 28.78 |
| 20 | ATOM | 4105 | CB  | ILE | A | 517 | 29.601 | 58.024 | 87.930 | 1.00 | 27.12 |
|    | ATOM | 4106 | CG1 | ILE | A | 517 | 29.225 | 56.610 | 88.312 | 1.00 | 29.40 |
|    | ATOM | 4107 | CG2 | ILE | A | 517 | 29.013 | 58.285 | 86.536 | 1.00 | 25.49 |
|    | ATOM | 4108 | CD1 | ILE | A | 517 | 29.305 | 55.665 | 87.105 | 1.00 | 34.77 |
|    | ATOM | 4109 | N   | LYS | A | 518 | 31.589 | 60.416 | 88.308 | 1.00 | 27.28 |
| 25 | ATOM | 4110 | CA  | LYS | A | 518 | 32.108 | 61.690 | 87.955 | 1.00 | 23.77 |
|    | ATOM | 4111 | C   | LYS | A | 518 | 33.558 | 61.482 | 87.485 | 1.00 | 24.03 |
|    | ATOM | 4112 | O   | LYS | A | 518 | 33.982 | 61.831 | 86.391 | 1.00 | 26.08 |
|    | ATOM | 4113 | CB  | LYS | A | 518 | 32.038 | 62.557 | 89.210 | 1.00 | 24.00 |
|    | ATOM | 4114 | CG  | LYS | A | 518 | 30.641 | 63.060 | 89.591 | 1.00 | 19.24 |
| 30 | ATOM | 4115 | CD  | LYS | A | 518 | 30.721 | 64.276 | 90.537 | 1.00 | 27.93 |
|    | ATOM | 4116 | CE  | LYS | A | 518 | 29.379 | 64.877 | 90.962 | 1.00 | 37.11 |
|    | ATOM | 4117 | NZ  | LYS | A | 518 | 28.924 | 65.988 | 90.104 | 1.00 | 52.30 |
|    | ATOM | 4118 | N   | ARG | A | 519 | 34.322 | 60.899 | 88.361 | 1.00 | 17.90 |
|    | ATOM | 4119 | CA  | ARG | A | 519 | 35.703 | 60.636 | 88.098 | 1.00 | 20.80 |
| 35 | ATOM | 4120 | C   | ARG | A | 519 | 35.862 | 59.874 | 86.802 | 1.00 | 28.98 |
|    | ATOM | 4121 | O   | ARG | A | 519 | 36.812 | 60.084 | 86.051 | 1.00 | 29.86 |
|    | ATOM | 4122 | CB  | ARG | A | 519 | 36.313 | 59.844 | 89.276 | 1.00 | 20.56 |
|    | ATOM | 4123 | CG  | ARG | A | 519 | 37.721 | 59.308 | 89.036 | 1.00 | 29.02 |
|    | ATOM | 4124 | CD  | ARG | A | 519 | 38.668 | 60.320 | 88.404 | 1.00 | 41.17 |
| 40 | ATOM | 4125 | NE  | ARG | A | 519 | 40.086 | 60.008 | 88.616 | 1.00 | 59.84 |
|    | ATOM | 4126 | CZ  | ARG | A | 519 | 41.076 | 60.858 | 88.349 | 1.00 | 50.77 |
|    | ATOM | 4127 | NH1 | ARG | A | 519 | 40.838 | 62.073 | 87.880 | 1.00 | 31.21 |
|    | ATOM | 4128 | NH2 | ARG | A | 519 | 42.329 | 60.486 | 88.543 | 1.00 | 31.86 |
|    | ATOM | 4129 | N   | MET | A | 520 | 34.937 | 58.956 | 86.565 | 1.00 | 25.08 |
| 45 | ATOM | 4130 | CA  | MET | A | 520 | 34.979 | 58.121 | 85.379 | 1.00 | 24.56 |
|    | ATOM | 4131 | C   | MET | A | 520 | 34.906 | 58.918 | 84.086 | 1.00 | 29.37 |
|    | ATOM | 4132 | O   | MET | A | 520 | 35.651 | 58.687 | 83.114 | 1.00 | 27.92 |
|    | ATOM | 4133 | CB  | MET | A | 520 | 33.905 | 57.007 | 85.442 | 1.00 | 26.98 |
|    | ATOM | 4134 | CG  | MET | A | 520 | 34.082 | 55.902 | 84.399 | 1.00 | 28.02 |
| 50 | ATOM | 4135 | SD  | MET | A | 520 | 32.830 | 54.591 | 84.479 | 1.00 | 27.87 |
|    | ATOM | 4136 | CE  | MET | A | 520 | 33.246 | 53.825 | 86.070 | 1.00 | 22.09 |
|    | ATOM | 4137 | N   | GLN | A | 521 | 33.982 | 59.864 | 84.067 | 1.00 | 28.32 |
|    | ATOM | 4138 | CA  | GLN | A | 521 | 33.838 | 60.672 | 82.886 | 1.00 | 28.34 |
|    | ATOM | 4139 | C   | GLN | A | 521 | 35.067 | 61.540 | 82.785 | 1.00 | 36.52 |
| 55 | ATOM | 4140 | O   | GLN | A | 521 | 35.514 | 61.879 | 81.707 | 1.00 | 35.87 |
|    | ATOM | 4141 | CB  | GLN | A | 521 | 32.514 | 61.451 | 82.863 | 1.00 | 28.34 |
|    | ATOM | 4142 | CG  | GLN | A | 521 | 32.564 | 62.774 | 82.079 | 1.00 | 9.68  |
|    | ATOM | 4143 | CD  | GLN | A | 521 | 32.890 | 62.572 | 80.616 | 1.00 | 27.55 |
|    | ATOM | 4144 | OE1 | GLN | A | 521 | 33.382 | 63.491 | 79.924 | 1.00 | 28.25 |
| 60 | ATOM | 4145 | NE2 | GLN | A | 521 | 32.657 | 61.368 | 80.142 | 1.00 | 25.70 |
|    | ATOM | 4146 | N   | GLU | A | 522 | 35.626 | 61.827 | 83.963 | 1.00 | 36.19 |
|    | ATOM | 4147 | CA  | GLU | A | 522 | 36.818 | 62.648 | 84.171 | 1.00 | 36.13 |
|    | ATOM | 4148 | C   | GLU | A | 522 | 38.136 | 62.046 | 83.662 | 1.00 | 42.48 |
|    | ATOM | 4149 | O   | GLU | A | 522 | 39.099 | 62.735 | 83.335 | 1.00 | 42.40 |
|    | ATOM | 4150 | CB  | GLU | A | 522 | 36.857 | 63.035 | 85.641 | 1.00 | 37.79 |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
|    | ATOM | 4151 | CG  | GLU | A | 522 | 38.233 | 63.196 | 86.273 | 1.00 | 58.85 |
|    | ATOM | 4152 | CD  | GLU | A | 522 | 38.046 | 64.040 | 87.493 | 1.00 | 73.64 |
|    | ATOM | 4153 | OE1 | GLU | A | 522 | 37.006 | 64.641 | 87.709 | 1.00 | 45.66 |
| 5  | ATOM | 4154 | OE2 | GLU | A | 522 | 39.081 | 64.037 | 88.289 | 1.00 | 47.91 |
|    | ATOM | 4155 | N   | VAL | A | 523 | 38.188 | 60.739 | 83.552 | 1.00 | 40.13 |
|    | ATOM | 4156 | CA  | VAL | A | 523 | 39.401 | 60.136 | 83.058 | 1.00 | 37.49 |
|    | ATOM | 4157 | C   | VAL | A | 523 | 39.205 | 59.351 | 81.778 | 1.00 | 38.88 |
|    | ATOM | 4158 | O   | VAL | A | 523 | 40.195 | 59.016 | 81.138 | 1.00 | 40.21 |
| 10 | ATOM | 4159 | CB  | VAL | A | 523 | 40.184 | 59.370 | 84.102 | 1.00 | 40.01 |
|    | ATOM | 4160 | CG1 | VAL | A | 523 | 40.231 | 60.165 | 85.413 | 1.00 | 39.12 |
|    | ATOM | 4161 | CG2 | VAL | A | 523 | 39.534 | 58.017 | 84.320 | 1.00 | 39.82 |
|    | ATOM | 4162 | N   | TYR | A | 524 | 37.952 | 59.048 | 81.379 | 1.00 | 30.35 |
|    | ATOM | 4163 | CA  | TYR | A | 524 | 37.801 | 58.330 | 80.114 | 1.00 | 28.11 |
|    | ATOM | 4164 | C   | TYR | A | 524 | 37.061 | 59.144 | 79.074 | 1.00 | 33.14 |
| 15 | ATOM | 4165 | O   | TYR | A | 524 | 37.076 | 58.802 | 77.908 | 1.00 | 35.84 |
|    | ATOM | 4166 | CB  | TYR | A | 524 | 37.281 | 56.878 | 80.119 | 1.00 | 25.56 |
|    | ATOM | 4167 | CG  | TYR | A | 524 | 37.941 | 55.960 | 81.111 | 1.00 | 20.87 |
|    | ATOM | 4168 | CD1 | TYR | A | 524 | 39.324 | 55.938 | 81.258 | 1.00 | 21.59 |
|    | ATOM | 4169 | CD2 | TYR | A | 524 | 37.170 | 55.083 | 81.879 | 1.00 | 19.80 |
| 20 | ATOM | 4170 | CE1 | TYR | A | 524 | 39.905 | 55.063 | 82.176 | 1.00 | 25.64 |
|    | ATOM | 4171 | CE2 | TYR | A | 524 | 37.731 | 54.227 | 82.827 | 1.00 | 18.61 |
|    | ATOM | 4172 | CZ  | TYR | A | 524 | 39.116 | 54.231 | 82.969 | 1.00 | 19.81 |
|    | ATOM | 4173 | OH  | TYR | A | 524 | 39.706 | 53.402 | 83.863 | 1.00 | 23.92 |
| 25 | ATOM | 4174 | N   | ASN | A | 525 | 36.416 | 60.221 | 79.496 | 1.00 | 25.98 |
|    | ATOM | 4175 | CA  | ASN | A | 525 | 35.687 | 61.088 | 78.588 | 1.00 | 25.01 |
|    | ATOM | 4176 | C   | ASN | A | 525 | 34.661 | 60.354 | 77.735 | 1.00 | 29.86 |
|    | ATOM | 4177 | O   | ASN | A | 525 | 34.533 | 60.535 | 76.499 | 1.00 | 29.39 |
|    | ATOM | 4178 | CB  | ASN | A | 525 | 36.637 | 61.922 | 77.739 | 1.00 | 29.55 |
|    | ATOM | 4179 | CG  | ASN | A | 525 | 35.949 | 62.980 | 76.894 | 1.00 | 30.32 |
| 30 | ATOM | 4180 | OD1 | ASN | A | 525 | 36.460 | 63.332 | 75.850 | 1.00 | 32.77 |
|    | ATOM | 4181 | ND2 | ASN | A | 525 | 34.822 | 63.527 | 77.344 | 1.00 | 13.80 |
|    | ATOM | 4182 | N   | PHE | A | 526 | 33.924 | 59.512 | 78.436 | 1.00 | 24.21 |
|    | ATOM | 4183 | CA  | PHE | A | 526 | 32.900 | 58.745 | 77.807 | 1.00 | 25.14 |
|    | ATOM | 4184 | C   | PHE | A | 526 | 31.846 | 59.631 | 77.214 | 1.00 | 31.74 |
| 35 | ATOM | 4185 | O   | PHE | A | 526 | 31.161 | 59.241 | 76.272 | 1.00 | 34.99 |
|    | ATOM | 4186 | CB  | PHE | A | 526 | 32.256 | 57.732 | 78.781 | 1.00 | 26.60 |
|    | ATOM | 4187 | CG  | PHE | A | 526 | 33.115 | 56.499 | 78.978 | 1.00 | 23.82 |
|    | ATOM | 4188 | CD1 | PHE | A | 526 | 34.017 | 56.080 | 78.000 | 1.00 | 25.00 |
|    | ATOM | 4189 | CD2 | PHE | A | 526 | 33.031 | 55.767 | 80.159 | 1.00 | 21.74 |
| 40 | ATOM | 4190 | CE1 | PHE | A | 526 | 34.783 | 54.927 | 78.173 | 1.00 | 27.63 |
|    | ATOM | 4191 | CE2 | PHE | A | 526 | 33.817 | 54.634 | 80.370 | 1.00 | 25.42 |
|    | ATOM | 4192 | CZ  | PHE | A | 526 | 34.683 | 54.202 | 79.364 | 1.00 | 25.28 |
|    | ATOM | 4193 | N   | ASN | A | 527 | 31.689 | 60.815 | 77.760 | 1.00 | 28.22 |
| 45 | ATOM | 4194 | CA  | ASN | A | 527 | 30.657 | 61.688 | 77.214 | 1.00 | 31.18 |
|    | ATOM | 4195 | C   | ASN | A | 527 | 30.884 | 62.046 | 75.744 | 1.00 | 33.17 |
|    | ATOM | 4196 | O   | ASN | A | 527 | 29.965 | 62.394 | 74.999 | 1.00 | 30.80 |
|    | ATOM | 4197 | CB  | ASN | A | 527 | 30.479 | 62.967 | 78.052 | 1.00 | 36.41 |
|    | ATOM | 4198 | CG  | ASN | A | 527 | 29.638 | 62.752 | 79.292 | 1.00 | 46.99 |
|    | ATOM | 4199 | OD1 | ASN | A | 527 | 29.647 | 63.571 | 80.209 | 1.00 | 36.82 |
| 50 | ATOM | 4200 | ND2 | ASN | A | 527 | 28.922 | 61.636 | 79.338 | 1.00 | 43.55 |
|    | ATOM | 4201 | N   | ALA | A | 528 | 32.136 | 61.947 | 75.348 | 1.00 | 27.46 |
|    | ATOM | 4202 | CA  | ALA | A | 528 | 32.581 | 62.278 | 74.005 | 1.00 | 26.48 |
|    | ATOM | 4203 | C   | ALA | A | 528 | 32.335 | 61.188 | 72.950 | 1.00 | 32.09 |
| 55 | ATOM | 4204 | O   | ALA | A | 528 | 32.420 | 61.404 | 71.753 | 1.00 | 32.09 |
|    | ATOM | 4205 | CB  | ALA | A | 528 | 34.076 | 62.584 | 74.105 | 1.00 | 26.04 |
|    | ATOM | 4206 | N   | ILE | A | 529 | 32.067 | 59.983 | 73.402 | 1.00 | 31.35 |
|    | ATOM | 4207 | CA  | ILE | A | 529 | 31.854 | 58.859 | 72.529 | 1.00 | 28.47 |
|    | ATOM | 4208 | C   | ILE | A | 529 | 30.492 | 58.904 | 71.887 | 1.00 | 35.96 |
|    | ATOM | 4209 | O   | ILE | A | 529 | 29.486 | 59.023 | 72.578 | 1.00 | 38.79 |
| 60 | ATOM | 4210 | CB  | ILE | A | 529 | 32.103 | 57.544 | 73.264 | 1.00 | 30.17 |
|    | ATOM | 4211 | CG1 | ILE | A | 529 | 33.622 | 57.291 | 73.392 | 1.00 | 31.37 |
|    | ATOM | 4212 | CG2 | ILE | A | 529 | 31.428 | 56.411 | 72.489 | 1.00 | 27.63 |
|    | ATOM | 4213 | CD1 | ILE | A | 529 | 34.059 | 56.515 | 74.635 | 1.00 | 33.41 |
|    | ATOM | 4214 | N   | ASN | A | 530 | 30.462 | 58.806 | 70.559 | 1.00 | 34.86 |



|    |      |      |     |     |   |     |        |        |        |      |        |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
|    | ATOM | 4215 | CA  | ASN | A | 530 | 29.196 | 58.841 | 69.852 | 1.00 | 36.44  |
|    | ATOM | 4216 | C   | ASN | A | 530 | 28.596 | 57.495 | 69.473 | 1.00 | 39.90  |
|    | ATOM | 4217 | O   | ASN | A | 530 | 27.452 | 57.437 | 69.043 | 1.00 | 41.37  |
| 5  | ATOM | 4218 | CB  | ASN | A | 530 | 28.951 | 60.044 | 68.928 | 1.00 | 51.44  |
|    | ATOM | 4219 | CG  | ASN | A | 530 | 28.461 | 61.253 | 69.732 | 1.00 | 100.00 |
|    | ATOM | 4220 | OD1 | ASN | A | 530 | 27.652 | 61.109 | 70.665 | 1.00 | 100.00 |
|    | ATOM | 4221 | ND2 | ASN | A | 530 | 28.955 | 62.442 | 69.392 | 1.00 | 91.39  |
|    | ATOM | 4222 | N   | ASN | A | 531 | 29.368 | 56.403 | 69.688 | 1.00 | 30.37  |
| 10 | ATOM | 4223 | CA  | ASN | A | 531 | 28.912 | 55.030 | 69.446 | 1.00 | 28.14  |
|    | ATOM | 4224 | C   | ASN | A | 531 | 27.696 | 54.753 | 70.360 | 1.00 | 32.80  |
|    | ATOM | 4225 | O   | ASN | A | 531 | 27.746 | 54.887 | 71.611 | 1.00 | 36.74  |
|    | ATOM | 4226 | CB  | ASN | A | 531 | 30.092 | 54.066 | 69.690 | 1.00 | 24.31  |
|    | ATOM | 4227 | CG  | ASN | A | 531 | 29.770 | 52.601 | 69.730 | 1.00 | 34.44  |
|    | ATOM | 4228 | OD1 | ASN | A | 531 | 28.795 | 52.182 | 70.359 | 1.00 | 36.49  |
| 15 | ATOM | 4229 | ND2 | ASN | A | 531 | 30.643 | 51.810 | 69.099 | 1.00 | 30.57  |
|    | ATOM | 4230 | N   | SER | A | 532 | 26.570 | 54.403 | 69.734 | 1.00 | 22.02  |
|    | ATOM | 4231 | CA  | SER | A | 532 | 25.325 | 54.183 | 70.459 | 1.00 | 19.67  |
|    | ATOM | 4232 | C   | SER | A | 532 | 25.323 | 53.208 | 71.627 | 1.00 | 26.15  |
|    | ATOM | 4233 | O   | SER | A | 532 | 24.767 | 53.475 | 72.680 | 1.00 | 26.64  |
| 20 | ATOM | 4234 | CB  | SER | A | 532 | 24.090 | 54.034 | 69.582 | 1.00 | 26.92  |
|    | ATOM | 4235 | OG  | SER | A | 532 | 24.294 | 53.211 | 68.452 | 1.00 | 23.59  |
|    | ATOM | 4236 | N   | GLU | A | 533 | 25.929 | 52.062 | 71.423 | 1.00 | 22.68  |
|    | ATOM | 4237 | CA  | GLU | A | 533 | 25.995 | 51.036 | 72.420 | 1.00 | 22.97  |
|    | ATOM | 4238 | C   | GLU | A | 533 | 26.677 | 51.569 | 73.635 | 1.00 | 30.48  |
| 25 | ATOM | 4239 | O   | GLU | A | 533 | 26.125 | 51.539 | 74.749 | 1.00 | 31.13  |
|    | ATOM | 4240 | CB  | GLU | A | 533 | 26.683 | 49.779 | 71.850 | 1.00 | 23.96  |
|    | ATOM | 4241 | CG  | GLU | A | 533 | 25.827 | 49.146 | 70.733 | 1.00 | 20.82  |
|    | ATOM | 4242 | CD  | GLU | A | 533 | 24.611 | 48.450 | 71.276 | 1.00 | 40.65  |
|    | ATOM | 4243 | OE1 | GLU | A | 533 | 24.432 | 48.256 | 72.476 | 1.00 | 36.25  |
| 30 | ATOM | 4244 | OE2 | GLU | A | 533 | 23.782 | 48.038 | 70.339 | 1.00 | 25.87  |
|    | ATOM | 4245 | N   | ILE | A | 534 | 27.872 | 52.101 | 73.392 | 1.00 | 26.20  |
|    | ATOM | 4246 | CA  | ILE | A | 534 | 28.622 | 52.672 | 74.484 | 1.00 | 26.32  |
|    | ATOM | 4247 | C   | ILE | A | 534 | 27.900 | 53.849 | 75.121 | 1.00 | 27.83  |
|    | ATOM | 4248 | O   | ILE | A | 534 | 27.697 | 53.911 | 76.326 | 1.00 | 26.54  |
| 35 | ATOM | 4249 | CB  | ILE | A | 534 | 30.051 | 53.022 | 74.102 | 1.00 | 29.16  |
|    | ATOM | 4250 | CG1 | ILE | A | 534 | 30.738 | 51.808 | 73.479 | 1.00 | 29.47  |
|    | ATOM | 4251 | CG2 | ILE | A | 534 | 30.801 | 53.458 | 75.353 | 1.00 | 28.28  |
|    | ATOM | 4252 | CD1 | ILE | A | 534 | 32.038 | 52.184 | 72.765 | 1.00 | 34.99  |
|    | ATOM | 4253 | N   | ARG | A | 535 | 27.480 | 54.805 | 74.320 | 1.00 | 24.30  |
| 40 | ATOM | 4254 | CA  | ARG | A | 535 | 26.804 | 55.898 | 74.949 | 1.00 | 22.51  |
|    | ATOM | 4255 | C   | ARG | A | 535 | 25.573 | 55.401 | 75.701 | 1.00 | 28.19  |
|    | ATOM | 4256 | O   | ARG | A | 535 | 25.212 | 55.808 | 76.791 | 1.00 | 32.61  |
|    | ATOM | 4257 | CB  | ARG | A | 535 | 26.457 | 56.942 | 73.913 | 1.00 | 24.83  |
|    | ATOM | 4258 | CG  | ARG | A | 535 | 25.970 | 58.229 | 74.541 | 1.00 | 21.49  |
| 45 | ATOM | 4259 | CD  | ARG | A | 535 | 25.327 | 59.183 | 73.554 | 1.00 | 13.79  |
|    | ATOM | 4260 | NE  | ARG | A | 535 | 25.194 | 60.457 | 74.213 | 1.00 | 31.38  |
|    | ATOM | 4261 | CZ  | ARG | A | 535 | 26.256 | 61.140 | 74.554 | 1.00 | 29.41  |
|    | ATOM | 4262 | NH1 | ARG | A | 535 | 27.463 | 60.677 | 74.259 | 1.00 | 26.45  |
|    | ATOM | 4263 | NH2 | ARG | A | 535 | 26.110 | 62.302 | 75.195 | 1.00 | 19.99  |
| 50 | ATOM | 4264 | N   | PHE | A | 536 | 24.911 | 54.466 | 75.126 | 1.00 | 23.44  |
|    | ATOM | 4265 | CA  | PHE | A | 536 | 23.740 | 53.980 | 75.770 | 1.00 | 22.05  |
|    | ATOM | 4266 | C   | PHE | A | 536 | 23.976 | 53.555 | 77.199 | 1.00 | 22.74  |
|    | ATOM | 4267 | O   | PHE | A | 536 | 23.349 | 54.113 | 78.105 | 1.00 | 22.06  |
|    | ATOM | 4268 | CB  | PHE | A | 536 | 23.117 | 52.865 | 74.919 | 1.00 | 23.17  |
| 55 | ATOM | 4269 | CG  | PHE | A | 536 | 22.040 | 52.153 | 75.658 | 1.00 | 21.92  |
|    | ATOM | 4270 | CD1 | PHE | A | 536 | 20.933 | 52.845 | 76.150 | 1.00 | 22.66  |
|    | ATOM | 4271 | CD2 | PHE | A | 536 | 22.145 | 50.783 | 75.882 | 1.00 | 23.25  |
|    | ATOM | 4272 | CE1 | PHE | A | 536 | 19.926 | 52.181 | 76.847 | 1.00 | 21.23  |
|    | ATOM | 4273 | CE2 | PHE | A | 536 | 21.147 | 50.101 | 76.576 | 1.00 | 24.70  |
| 60 | ATOM | 4274 | CZ  | PHE | A | 536 | 20.047 | 50.811 | 77.065 | 1.00 | 20.57  |
|    | ATOM | 4275 | N   | ARG | A | 537 | 24.863 | 52.560 | 77.364 | 1.00 | 18.22  |
|    | ATOM | 4276 | CA  | ARG | A | 537 | 25.239 | 51.995 | 78.665 | 1.00 | 19.20  |
|    | ATOM | 4277 | C   | ARG | A | 537 | 25.932 | 52.963 | 79.618 | 1.00 | 27.62  |
|    | ATOM | 4278 | O   | ARG | A | 537 | 25.803 | 52.845 | 80.837 | 1.00 | 26.73  |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
|    | ATOM | 4279 | CB  | ARG | A | 537 | 26.035 | 50.709 | 78.556 | 1.00 | 18.91 |
|    | ATOM | 4280 | CG  | ARG | A | 537 | 25.318 | 49.656 | 77.708 | 1.00 | 16.55 |
|    | ATOM | 4281 | CD  | ARG | A | 537 | 26.181 | 48.426 | 77.387 | 1.00 | 21.58 |
| 5  | ATOM | 4282 | NE  | ARG | A | 537 | 25.341 | 47.357 | 76.886 | 1.00 | 28.42 |
|    | ATOM | 4283 | CZ  | ARG | A | 537 | 25.060 | 47.206 | 75.609 | 1.00 | 18.29 |
|    | ATOM | 4284 | NH1 | ARG | A | 537 | 25.569 | 48.004 | 74.703 | 1.00 | 22.46 |
|    | ATOM | 4285 | NH2 | ARG | A | 537 | 24.240 | 46.236 | 75.224 | 1.00 | 25.22 |
|    | ATOM | 4286 | N   | TRP | A | 538 | 26.668 | 53.930 | 79.064 | 1.00 | 24.21 |
| 10 | ATOM | 4287 | CA  | TRP | A | 538 | 27.337 | 54.918 | 79.867 | 1.00 | 22.11 |
|    | ATOM | 4288 | C   | TRP | A | 538 | 26.274 | 55.719 | 80.550 | 1.00 | 28.09 |
|    | ATOM | 4289 | O   | TRP | A | 538 | 26.320 | 55.951 | 81.741 | 1.00 | 27.39 |
|    | ATOM | 4290 | CB  | TRP | A | 538 | 28.064 | 55.888 | 78.949 | 1.00 | 20.48 |
|    | ATOM | 4291 | CG  | TRP | A | 538 | 28.606 | 57.157 | 79.580 | 1.00 | 21.29 |
| 15 | ATOM | 4292 | CD1 | TRP | A | 538 | 28.641 | 58.345 | 78.968 | 1.00 | 22.86 |
|    | ATOM | 4293 | CD2 | TRP | A | 538 | 29.286 | 57.352 | 80.845 | 1.00 | 21.79 |
|    | ATOM | 4294 | NE1 | TRP | A | 538 | 29.228 | 59.270 | 79.769 | 1.00 | 22.70 |
|    | ATOM | 4295 | CE2 | TRP | A | 538 | 29.643 | 58.696 | 80.911 | 1.00 | 24.79 |
|    | ATOM | 4296 | CE3 | TRP | A | 538 | 29.574 | 56.535 | 81.946 | 1.00 | 23.35 |
| 20 | ATOM | 4297 | CZ2 | TRP | A | 538 | 30.280 | 59.248 | 82.025 | 1.00 | 25.89 |
|    | ATOM | 4298 | CZ3 | TRP | A | 538 | 30.203 | 57.056 | 83.046 | 1.00 | 23.35 |
|    | ATOM | 4299 | CH2 | TRP | A | 538 | 30.562 | 58.405 | 83.081 | 1.00 | 24.89 |
|    | ATOM | 4300 | N   | LEU | A | 539 | 25.303 | 56.161 | 79.758 | 1.00 | 27.31 |
|    | ATOM | 4301 | CA  | LEU | A | 539 | 24.229 | 56.974 | 80.306 | 1.00 | 27.18 |
| 25 | ATOM | 4302 | C   | LEU | A | 539 | 23.369 | 56.245 | 81.332 | 1.00 | 28.25 |
|    | ATOM | 4303 | O   | LEU | A | 539 | 22.857 | 56.822 | 82.266 | 1.00 | 27.19 |
|    | ATOM | 4304 | CB  | LEU | A | 539 | 23.428 | 57.812 | 79.262 | 1.00 | 26.37 |
|    | ATOM | 4305 | CG  | LEU | A | 539 | 24.269 | 58.682 | 78.279 | 1.00 | 25.71 |
|    | ATOM | 4306 | CD1 | LEU | A | 539 | 23.369 | 59.424 | 77.290 | 1.00 | 21.79 |
| 30 | ATOM | 4307 | CD2 | LEU | A | 539 | 25.146 | 59.680 | 79.011 | 1.00 | 23.51 |
|    | ATOM | 4308 | N   | ARG | A | 540 | 23.199 | 54.960 | 81.188 | 1.00 | 27.56 |
|    | ATOM | 4309 | CA  | ARG | A | 540 | 22.390 | 54.283 | 82.170 | 1.00 | 26.88 |
|    | ATOM | 4310 | C   | ARG | A | 540 | 23.145 | 54.229 | 83.453 | 1.00 | 31.82 |
|    | ATOM | 4311 | O   | ARG | A | 540 | 22.618 | 54.448 | 84.539 | 1.00 | 32.72 |
| 35 | ATOM | 4312 | CB  | ARG | A | 540 | 22.034 | 52.888 | 81.732 | 1.00 | 24.48 |
|    | ATOM | 4313 | CG  | ARG | A | 540 | 21.447 | 52.885 | 80.331 | 1.00 | 32.96 |
|    | ATOM | 4314 | CD  | ARG | A | 540 | 20.695 | 51.597 | 80.090 | 1.00 | 33.19 |
|    | ATOM | 4315 | NE  | ARG | A | 540 | 19.660 | 51.414 | 81.085 | 1.00 | 33.95 |
|    | ATOM | 4316 | CZ  | ARG | A | 540 | 19.151 | 50.242 | 81.409 | 1.00 | 30.83 |
| 40 | ATOM | 4317 | NH1 | ARG | A | 540 | 19.564 | 49.132 | 80.849 | 1.00 | 25.37 |
|    | ATOM | 4318 | NH2 | ARG | A | 540 | 18.186 | 50.186 | 82.317 | 1.00 | 30.30 |
|    | ATOM | 4319 | N   | LEU | A | 541 | 24.414 | 53.948 | 83.318 | 1.00 | 28.93 |
|    | ATOM | 4320 | CA  | LEU | A | 541 | 25.239 | 53.895 | 84.505 | 1.00 | 26.36 |
|    | ATOM | 4321 | C   | LEU | A | 541 | 25.036 | 55.210 | 85.277 | 1.00 | 31.00 |
| 45 | ATOM | 4322 | O   | LEU | A | 541 | 24.632 | 55.246 | 86.439 | 1.00 | 31.62 |
|    | ATOM | 4323 | CB  | LEU | A | 541 | 26.702 | 53.586 | 84.094 | 1.00 | 23.61 |
|    | ATOM | 4324 | CG  | LEU | A | 541 | 27.730 | 53.533 | 85.212 | 1.00 | 24.67 |
|    | ATOM | 4325 | CD1 | LEU | A | 541 | 27.387 | 52.411 | 86.190 | 1.00 | 25.02 |
|    | ATOM | 4326 | CD2 | LEU | A | 541 | 29.098 | 53.245 | 84.621 | 1.00 | 19.31 |
| 50 | ATOM | 4327 | N   | CYS | A | 542 | 25.254 | 56.307 | 84.570 | 1.00 | 30.52 |
|    | ATOM | 4328 | CA  | CYS | A | 542 | 25.115 | 57.661 | 85.105 | 1.00 | 31.76 |
|    | ATOM | 4329 | C   | CYS | A | 542 | 23.808 | 57.996 | 85.805 | 1.00 | 32.71 |
|    | ATOM | 4330 | O   | CYS | A | 542 | 23.801 | 58.536 | 86.914 | 1.00 | 33.97 |
|    | ATOM | 4331 | CB  | CYS | A | 542 | 25.461 | 58.744 | 84.073 | 1.00 | 31.30 |
| 55 | ATOM | 4332 | SG  | CYS | A | 542 | 27.085 | 58.488 | 83.347 | 1.00 | 34.39 |
|    | ATOM | 4333 | N   | ILE | A | 543 | 22.711 | 57.708 | 85.125 | 1.00 | 25.61 |
|    | ATOM | 4334 | CA  | ILE | A | 543 | 21.382 | 57.982 | 85.643 | 1.00 | 23.12 |
|    | ATOM | 4335 | C   | ILE | A | 543 | 21.199 | 57.161 | 86.885 | 1.00 | 30.15 |
|    | ATOM | 4336 | O   | ILE | A | 543 | 20.900 | 57.645 | 87.972 | 1.00 | 30.73 |
| 60 | ATOM | 4337 | CB  | ILE | A | 543 | 20.340 | 57.627 | 84.585 | 1.00 | 23.75 |
|    | ATOM | 4338 | CG1 | ILE | A | 543 | 20.369 | 58.664 | 83.468 | 1.00 | 24.09 |
|    | ATOM | 4339 | CG2 | ILE | A | 543 | 18.955 | 57.572 | 85.182 | 1.00 | 22.99 |
|    | ATOM | 4340 | CD1 | ILE | A | 543 | 20.386 | 60.109 | 83.982 | 1.00 | 27.34 |
|    | ATOM | 4341 | N   | GLN | A | 544 | 21.440 | 55.884 | 86.695 | 1.00 | 27.99 |
|    | ATOM | 4342 | CA  | GLN | A | 544 | 21.320 | 54.929 | 87.756 | 1.00 | 25.72 |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
|    | ATOM | 4343 | C   | GLN | A | 544 | 22.243 | 55.269 | 88.901 | 1.00 | 26.34 |
|    | ATOM | 4344 | O   | GLN | A | 544 | 22.029 | 54.826 | 90.014 | 1.00 | 26.24 |
|    | ATOM | 4345 | CB  | GLN | A | 544 | 21.562 | 53.512 | 87.210 | 1.00 | 26.76 |
| 5  | ATOM | 4346 | CG  | GLN | A | 544 | 20.355 | 52.955 | 86.432 | 1.00 | 17.74 |
|    | ATOM | 4347 | CD  | GLN | A | 544 | 20.598 | 51.604 | 85.743 | 1.00 | 32.62 |
|    | ATOM | 4348 | OE1 | GLN | A | 544 | 20.326 | 51.432 | 84.551 | 1.00 | 38.66 |
|    | ATOM | 4349 | NE2 | GLN | A | 544 | 21.063 | 50.627 | 86.494 | 1.00 | 14.93 |
|    | ATOM | 4350 | N   | SER | A | 545 | 23.286 | 56.033 | 88.625 | 1.00 | 21.73 |
| 10 | ATOM | 4351 | CA  | SER | A | 545 | 24.187 | 56.392 | 89.685 | 1.00 | 22.42 |
|    | ATOM | 4352 | C   | SER | A | 545 | 23.819 | 57.726 | 90.287 | 1.00 | 33.67 |
|    | ATOM | 4353 | O   | SER | A | 545 | 24.567 | 58.257 | 91.133 | 1.00 | 37.22 |
|    | ATOM | 4354 | CB  | SER | A | 545 | 25.646 | 56.322 | 89.338 | 1.00 | 21.57 |
|    | ATOM | 4355 | OG  | SER | A | 545 | 25.980 | 54.968 | 89.163 | 1.00 | 31.72 |
| 15 | ATOM | 4356 | N   | LYS | A | 546 | 22.662 | 58.251 | 89.841 | 1.00 | 23.09 |
|    | ATOM | 4357 | CA  | LYS | A | 546 | 22.135 | 59.490 | 90.356 | 1.00 | 20.79 |
|    | ATOM | 4358 | C   | LYS | A | 546 | 22.887 | 60.738 | 89.961 | 1.00 | 27.55 |
|    | ATOM | 4359 | O   | LYS | A | 546 | 23.001 | 61.655 | 90.771 | 1.00 | 27.95 |
|    | ATOM | 4360 | CB  | LYS | A | 546 | 22.126 | 59.449 | 91.881 | 1.00 | 21.71 |
| 20 | ATOM | 4361 | CG  | LYS | A | 546 | 21.498 | 58.195 | 92.484 | 1.00 | 15.90 |
|    | ATOM | 4362 | CD  | LYS | A | 546 | 20.245 | 57.814 | 91.731 | 1.00 | 39.84 |
|    | ATOM | 4363 | CE  | LYS | A | 546 | 19.355 | 56.850 | 92.498 | 1.00 | 45.16 |
|    | ATOM | 4364 | NZ  | LYS | A | 546 | 18.197 | 56.399 | 91.704 | 1.00 | 40.14 |
|    | ATOM | 4365 | N   | TRP | A | 547 | 23.414 | 60.776 | 88.753 | 1.00 | 23.26 |
| 25 | ATOM | 4366 | CA  | TRP | A | 547 | 24.141 | 61.931 | 88.289 | 1.00 | 21.90 |
|    | ATOM | 4367 | C   | TRP | A | 547 | 23.221 | 62.901 | 87.570 | 1.00 | 29.82 |
|    | ATOM | 4368 | O   | TRP | A | 547 | 22.808 | 62.679 | 86.432 | 1.00 | 34.91 |
|    | ATOM | 4369 | CB  | TRP | A | 547 | 25.262 | 61.500 | 87.361 | 1.00 | 21.04 |
|    | ATOM | 4370 | CG  | TRP | A | 547 | 26.254 | 62.591 | 87.206 | 1.00 | 22.57 |
|    | ATOM | 4371 | CD1 | TRP | A | 547 | 26.224 | 63.769 | 87.844 | 1.00 | 25.87 |
| 30 | ATOM | 4372 | CD2 | TRP | A | 547 | 27.437 | 62.588 | 86.417 | 1.00 | 23.40 |
|    | ATOM | 4373 | NE1 | TRP | A | 547 | 27.316 | 64.511 | 87.517 | 1.00 | 25.64 |
|    | ATOM | 4374 | CE2 | TRP | A | 547 | 28.081 | 63.819 | 86.635 | 1.00 | 27.46 |
|    | ATOM | 4375 | CE3 | TRP | A | 547 | 28.014 | 61.668 | 85.547 | 1.00 | 26.21 |
|    | ATOM | 4376 | CZ2 | TRP | A | 547 | 29.279 | 64.162 | 85.995 | 1.00 | 27.44 |
| 35 | ATOM | 4377 | CZ3 | TRP | A | 547 | 29.195 | 62.009 | 84.923 | 1.00 | 28.70 |
|    | ATOM | 4378 | CH2 | TRP | A | 547 | 29.822 | 63.236 | 85.138 | 1.00 | 28.41 |
|    | ATOM | 4379 | N   | GLU | A | 548 | 22.888 | 63.995 | 88.227 | 1.00 | 22.95 |
|    | ATOM | 4380 | CA  | GLU | A | 548 | 21.979 | 64.970 | 87.649 | 1.00 | 20.70 |
| 40 | ATOM | 4381 | C   | GLU | A | 548 | 22.419 | 65.473 | 86.305 | 1.00 | 28.32 |
|    | ATOM | 4382 | O   | GLU | A | 548 | 21.598 | 65.735 | 85.391 | 1.00 | 29.41 |
|    | ATOM | 4383 | CB  | GLU | A | 548 | 21.635 | 66.144 | 88.607 | 1.00 | 22.45 |
|    | ATOM | 4384 | CG  | GLU | A | 548 | 20.884 | 65.709 | 89.919 | 1.00 | 30.56 |
|    | ATOM | 4385 | CD  | GLU | A | 548 | 20.337 | 66.848 | 90.765 | 1.00 | 59.35 |
|    | ATOM | 4386 | OE1 | GLU | A | 548 | 20.336 | 68.021 | 90.413 | 1.00 | 81.52 |
| 45 | ATOM | 4387 | OE2 | GLU | A | 548 | 19.888 | 66.450 | 91.925 | 1.00 | 57.05 |
|    | ATOM | 4388 | N   | ASP | A | 549 | 23.728 | 65.661 | 86.201 | 1.00 | 24.72 |
|    | ATOM | 4389 | CA  | ASP | A | 549 | 24.276 | 66.190 | 84.981 | 1.00 | 21.48 |
|    | ATOM | 4390 | C   | ASP | A | 549 | 23.914 | 65.359 | 83.795 | 1.00 | 30.08 |
| 50 | ATOM | 4391 | O   | ASP | A | 549 | 23.760 | 65.869 | 82.697 | 1.00 | 32.05 |
|    | ATOM | 4392 | CB  | ASP | A | 549 | 25.775 | 66.480 | 85.048 | 1.00 | 21.28 |
|    | ATOM | 4393 | CG  | ASP | A | 549 | 26.076 | 67.463 | 86.130 | 1.00 | 37.74 |
|    | ATOM | 4394 | OD1 | ASP | A | 549 | 25.432 | 68.479 | 86.297 | 1.00 | 48.21 |
|    | ATOM | 4395 | OD2 | ASP | A | 549 | 27.076 | 67.115 | 86.882 | 1.00 | 46.51 |
| 55 | ATOM | 4396 | N   | ALA | A | 550 | 23.766 | 64.073 | 84.032 | 1.00 | 27.68 |
|    | ATOM | 4397 | CA  | ALA | A | 550 | 23.445 | 63.133 | 82.965 | 1.00 | 26.74 |
|    | ATOM | 4398 | C   | ALA | A | 550 | 22.019 | 63.171 | 82.431 | 1.00 | 32.35 |
|    | ATOM | 4399 | O   | ALA | A | 550 | 21.745 | 62.615 | 81.361 | 1.00 | 31.95 |
|    | ATOM | 4400 | CB  | ALA | A | 550 | 23.812 | 61.713 | 83.372 | 1.00 | 25.48 |
| 60 | ATOM | 4401 | N   | ILE | A | 551 | 21.123 | 63.795 | 83.192 | 1.00 | 28.71 |
|    | ATOM | 4402 | CA  | ILE | A | 551 | 19.716 | 63.882 | 82.832 | 1.00 | 28.20 |
|    | ATOM | 4403 | C   | ILE | A | 551 | 19.461 | 64.355 | 81.411 | 1.00 | 32.04 |
|    | ATOM | 4404 | O   | ILE | A | 551 | 18.833 | 63.679 | 80.619 | 1.00 | 31.75 |
|    | ATOM | 4405 | CB  | ILE | A | 551 | 18.876 | 64.641 | 83.868 | 1.00 | 30.29 |
|    | ATOM | 4406 | CG1 | ILE | A | 551 | 19.038 | 63.985 | 85.226 | 1.00 | 31.50 |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
|    | ATOM | 4407 | CG2 | ILE | A | 551 | 17.391 | 64.661 | 83.475 | 1.00 | 24.75 |
|    | ATOM | 4408 | CD1 | ILE | A | 551 | 18.072 | 64.561 | 86.253 | 1.00 | 31.62 |
|    | ATOM | 4409 | N   | PRO | A | 552 | 19.969 | 65.529 | 81.099 | 1.00 | 33.75 |
| 5  | ATOM | 4410 | CA  | PRO | A | 552 | 19.793 | 66.121 | 79.796 | 1.00 | 32.60 |
|    | ATOM | 4411 | C   | PRO | A | 552 | 20.240 | 65.224 | 78.669 | 1.00 | 30.34 |
|    | ATOM | 4412 | O   | PRO | A | 552 | 19.583 | 65.119 | 77.622 | 1.00 | 27.23 |
|    | ATOM | 4413 | CB  | PRO | A | 552 | 20.659 | 67.383 | 79.787 | 1.00 | 34.45 |
|    | ATOM | 4414 | CG  | PRO | A | 552 | 21.348 | 67.500 | 81.139 | 1.00 | 38.39 |
| 10 | ATOM | 4415 | CD  | PRO | A | 552 | 20.934 | 66.296 | 81.950 | 1.00 | 34.48 |
|    | ATOM | 4416 | N   | LEU | A | 553 | 21.391 | 64.616 | 78.891 | 1.00 | 23.74 |
|    | ATOM | 4417 | CA  | LEU | A | 553 | 21.997 | 63.727 | 77.931 | 1.00 | 22.72 |
|    | ATOM | 4418 | C   | LEU | A | 553 | 21.138 | 62.522 | 77.670 | 1.00 | 32.68 |
|    | ATOM | 4419 | O   | LEU | A | 553 | 21.015 | 62.087 | 76.523 | 1.00 | 35.70 |
| 15 | ATOM | 4420 | CB  | LEU | A | 553 | 23.362 | 63.281 | 78.439 | 1.00 | 21.57 |
|    | ATOM | 4421 | CG  | LEU | A | 553 | 24.196 | 64.496 | 78.818 | 1.00 | 24.02 |
|    | ATOM | 4422 | CD1 | LEU | A | 553 | 25.608 | 64.071 | 79.174 | 1.00 | 19.59 |
|    | ATOM | 4423 | CD2 | LEU | A | 553 | 24.188 | 65.479 | 77.630 | 1.00 | 18.60 |
|    | ATOM | 4424 | N   | ALA | A | 554 | 20.563 | 61.973 | 78.754 | 1.00 | 30.05 |
| 20 | ATOM | 4425 | CA  | ALA | A | 554 | 19.726 | 60.779 | 78.669 | 1.00 | 27.72 |
|    | ATOM | 4426 | C   | ALA | A | 554 | 18.432 | 61.107 | 77.988 | 1.00 | 36.03 |
|    | ATOM | 4427 | O   | ALA | A | 554 | 17.944 | 60.332 | 77.163 | 1.00 | 37.08 |
|    | ATOM | 4428 | CB  | ALA | A | 554 | 19.475 | 60.165 | 80.017 | 1.00 | 26.78 |
|    | ATOM | 4429 | N   | LEU | A | 555 | 17.898 | 62.283 | 78.320 | 1.00 | 29.70 |
| 25 | ATOM | 4430 | CA  | LEU | A | 555 | 16.644 | 62.724 | 77.720 | 1.00 | 28.32 |
|    | ATOM | 4431 | C   | LEU | A | 555 | 16.803 | 62.902 | 76.229 | 1.00 | 29.19 |
|    | ATOM | 4432 | O   | LEU | A | 555 | 15.970 | 62.506 | 75.385 | 1.00 | 26.13 |
|    | ATOM | 4433 | CB  | LEU | A | 555 | 16.110 | 64.027 | 78.342 | 1.00 | 28.26 |
|    | ATOM | 4434 | CG  | LEU | A | 555 | 15.371 | 63.814 | 79.666 | 1.00 | 32.76 |
| 30 | ATOM | 4435 | CD1 | LEU | A | 555 | 15.360 | 65.118 | 80.464 | 1.00 | 34.66 |
|    | ATOM | 4436 | CD2 | LEU | A | 555 | 13.938 | 63.334 | 79.427 | 1.00 | 27.50 |
|    | ATOM | 4437 | N   | LYS | A | 556 | 17.922 | 63.524 | 75.950 | 1.00 | 28.45 |
|    | ATOM | 4438 | CA  | LYS | A | 556 | 18.325 | 63.839 | 74.615 | 1.00 | 28.76 |
|    | ATOM | 4439 | C   | LYS | A | 556 | 18.369 | 62.591 | 73.800 | 1.00 | 35.11 |
| 35 | ATOM | 4440 | O   | LYS | A | 556 | 17.670 | 62.491 | 72.796 | 1.00 | 41.80 |
|    | ATOM | 4441 | CB  | LYS | A | 556 | 19.645 | 64.592 | 74.599 | 1.00 | 31.79 |
|    | ATOM | 4442 | CG  | LYS | A | 556 | 20.101 | 65.139 | 73.250 | 1.00 | 63.55 |
|    | ATOM | 4443 | CD  | LYS | A | 556 | 21.585 | 65.518 | 73.254 | 1.00 | 81.77 |
|    | ATOM | 4444 | CE  | LYS | A | 556 | 22.046 | 66.270 | 72.011 | 1.00 | 79.68 |
| 40 | ATOM | 4445 | NZ  | LYS | A | 556 | 23.239 | 65.661 | 71.401 | 1.00 | 73.00 |
|    | ATOM | 4446 | N   | MET | A | 557 | 19.154 | 61.623 | 74.248 | 1.00 | 26.96 |
|    | ATOM | 4447 | CA  | MET | A | 557 | 19.305 | 60.364 | 73.514 | 1.00 | 23.97 |
|    | ATOM | 4448 | C   | MET | A | 557 | 18.033 | 59.553 | 73.287 | 1.00 | 30.96 |
|    | ATOM | 4449 | O   | MET | A | 557 | 17.811 | 58.907 | 72.263 | 1.00 | 23.24 |
| 45 | ATOM | 4450 | CB  | MET | A | 557 | 20.401 | 59.488 | 74.104 | 1.00 | 24.89 |
|    | ATOM | 4451 | CG  | MET | A | 557 | 20.533 | 58.163 | 73.368 | 1.00 | 29.37 |
|    | ATOM | 4452 | SD  | MET | A | 557 | 22.029 | 57.276 | 73.864 | 1.00 | 33.21 |
|    | ATOM | 4453 | CE  | MET | A | 557 | 21.939 | 55.812 | 72.793 | 1.00 | 30.16 |
|    | ATOM | 4454 | N   | ALA | A | 558 | 17.203 | 59.568 | 74.287 | 1.00 | 33.42 |
| 50 | ATOM | 4455 | CA  | ALA | A | 558 | 16.000 | 58.816 | 74.194 | 1.00 | 33.03 |
|    | ATOM | 4456 | C   | ALA | A | 558 | 15.042 | 59.345 | 73.163 | 1.00 | 38.12 |
|    | ATOM | 4457 | O   | ALA | A | 558 | 14.349 | 58.568 | 72.543 | 1.00 | 37.09 |
|    | ATOM | 4458 | CB  | ALA | A | 558 | 15.317 | 58.780 | 75.553 | 1.00 | 32.89 |
|    | ATOM | 4459 | N   | THR | A | 559 | 14.994 | 60.665 | 73.032 | 1.00 | 36.76 |
| 55 | ATOM | 4460 | CA  | THR | A | 559 | 14.067 | 61.326 | 72.144 | 1.00 | 36.43 |
|    | ATOM | 4461 | C   | THR | A | 559 | 14.588 | 61.590 | 70.794 | 1.00 | 41.71 |
|    | ATOM | 4462 | O   | THR | A | 559 | 13.788 | 61.768 | 69.891 | 1.00 | 44.66 |
|    | ATOM | 4463 | CB  | THR | A | 559 | 13.615 | 62.705 | 72.694 | 1.00 | 43.70 |
|    | ATOM | 4464 | OG1 | THR | A | 559 | 14.728 | 63.545 | 72.957 | 1.00 | 38.88 |
| 60 | ATOM | 4465 | CG2 | THR | A | 559 | 12.764 | 62.549 | 73.942 | 1.00 | 44.95 |
|    | ATOM | 4466 | N   | GLU | A | 560 | 15.897 | 61.695 | 70.674 | 1.00 | 37.38 |
|    | ATOM | 4467 | CA  | GLU | A | 560 | 16.495 | 62.018 | 69.395 | 1.00 | 36.51 |
|    | ATOM | 4468 | C   | GLU | A | 560 | 16.652 | 60.846 | 68.448 | 1.00 | 40.11 |
|    | ATOM | 4469 | O   | GLU | A | 560 | 17.003 | 61.052 | 67.300 | 1.00 | 43.23 |
|    | ATOM | 4470 | CB  | GLU | A | 560 | 17.799 | 62.820 | 69.519 | 1.00 | 38.13 |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
|    | ATOM | 4471 | CG  | GLU | A | 560 | 17.653 | 64.142 | 70.292 | 1.00 | 54.29 |
|    | ATOM | 4472 | CD  | GLU | A | 560 | 18.857 | 65.043 | 70.127 | 1.00 | 78.42 |
|    | ATOM | 4473 | OE1 | GLU | A | 560 | 19.960 | 64.639 | 69.812 | 1.00 | 32.69 |
| 5  | ATOM | 4474 | OE2 | GLU | A | 560 | 18.593 | 66.303 | 70.380 | 1.00 | 85.90 |
|    | ATOM | 4475 | N   | GLN | A | 561 | 16.425 | 59.627 | 68.955 | 1.00 | 30.45 |
|    | ATOM | 4476 | CA  | GLN | A | 561 | 16.467 | 58.356 | 68.230 | 1.00 | 22.57 |
|    | ATOM | 4477 | C   | GLN | A | 561 | 15.398 | 57.523 | 68.878 | 1.00 | 26.95 |
|    | ATOM | 4478 | O   | GLN | A | 561 | 14.978 | 57.814 | 69.975 | 1.00 | 27.79 |
| 10 | ATOM | 4479 | CB  | GLN | A | 561 | 17.829 | 57.661 | 68.128 | 1.00 | 20.64 |
|    | ATOM | 4480 | CG  | GLN | A | 561 | 18.470 | 57.290 | 69.491 | 1.00 | 22.59 |
|    | ATOM | 4481 | CD  | GLN | A | 561 | 17.802 | 56.121 | 70.184 | 1.00 | 28.22 |
|    | ATOM | 4482 | OE1 | GLN | A | 561 | 17.524 | 56.156 | 71.400 | 1.00 | 37.44 |
|    | ATOM | 4483 | NE2 | GLN | A | 561 | 17.556 | 55.069 | 69.419 | 1.00 | 31.92 |
| 15 | ATOM | 4484 | N   | GLY | A | 562 | 14.888 | 56.535 | 68.209 | 1.00 | 26.16 |
|    | ATOM | 4485 | CA  | GLY | A | 562 | 13.801 | 55.810 | 68.858 | 1.00 | 27.83 |
|    | ATOM | 4486 | C   | GLY | A | 562 | 13.932 | 54.320 | 68.761 | 1.00 | 41.56 |
|    | ATOM | 4487 | O   | GLY | A | 562 | 12.936 | 53.614 | 68.677 | 1.00 | 45.37 |
|    | ATOM | 4488 | N   | ARG | A | 563 | 15.171 | 53.864 | 68.742 | 1.00 | 37.40 |
| 20 | ATOM | 4489 | CA  | ARG | A | 563 | 15.457 | 52.453 | 68.689 | 1.00 | 34.41 |
|    | ATOM | 4490 | C   | ARG | A | 563 | 15.121 | 51.939 | 70.109 | 1.00 | 39.48 |
|    | ATOM | 4491 | O   | ARG | A | 563 | 15.832 | 52.221 | 71.087 | 1.00 | 40.29 |
|    | ATOM | 4492 | CB  | ARG | A | 563 | 16.932 | 52.231 | 68.284 | 1.00 | 18.23 |
|    | ATOM | 4493 | CG  | ARG | A | 563 | 17.309 | 50.755 | 68.169 | 1.00 | 20.07 |
| 25 | ATOM | 4494 | CD  | ARG | A | 563 | 18.779 | 50.514 | 68.512 | 1.00 | 25.07 |
|    | ATOM | 4495 | NE  | ARG | A | 563 | 19.234 | 49.139 | 68.320 | 1.00 | 25.66 |
|    | ATOM | 4496 | CZ  | ARG | A | 563 | 20.425 | 48.891 | 67.821 | 1.00 | 26.35 |
|    | ATOM | 4497 | NH1 | ARG | A | 563 | 21.257 | 49.860 | 67.430 | 1.00 | 12.96 |
|    | ATOM | 4498 | NH2 | ARG | A | 563 | 20.804 | 47.636 | 67.656 | 1.00 | 30.31 |
| 30 | ATOM | 4499 | N   | MET | A | 564 | 13.989 | 51.228 | 70.239 | 1.00 | 33.12 |
|    | ATOM | 4500 | CA  | MET | A | 564 | 13.487 | 50.695 | 71.526 | 1.00 | 31.84 |
|    | ATOM | 4501 | C   | MET | A | 564 | 14.565 | 50.247 | 72.532 | 1.00 | 31.42 |
|    | ATOM | 4502 | O   | MET | A | 564 | 14.494 | 50.501 | 73.744 | 1.00 | 25.72 |
|    | ATOM | 4503 | CB  | MET | A | 564 | 12.323 | 49.682 | 71.365 | 1.00 | 32.45 |
| 35 | ATOM | 4504 | CG  | MET | A | 564 | 11.196 | 50.225 | 70.487 | 1.00 | 35.78 |
|    | ATOM | 4505 | SD  | MET | A | 564 | 9.695  | 49.205 | 70.533 | 1.00 | 40.85 |
|    | ATOM | 4506 | CE  | MET | A | 564 | 10.177 | 47.892 | 69.382 | 1.00 | 35.87 |
|    | ATOM | 4507 | N   | LYS | A | 565 | 15.562 | 49.581 | 71.966 | 1.00 | 31.68 |
|    | ATOM | 4508 | CA  | LYS | A | 565 | 16.699 | 49.041 | 72.668 | 1.00 | 29.04 |
| 40 | ATOM | 4509 | C   | LYS | A | 565 | 17.281 | 50.089 | 73.562 | 1.00 | 26.36 |
|    | ATOM | 4510 | O   | LYS | A | 565 | 17.648 | 49.782 | 74.673 | 1.00 | 21.19 |
|    | ATOM | 4511 | CB  | LYS | A | 565 | 17.747 | 48.494 | 71.697 | 1.00 | 29.06 |
|    | ATOM | 4512 | CG  | LYS | A | 565 | 18.864 | 47.715 | 72.359 | 1.00 | 23.89 |
|    | ATOM | 4513 | CD  | LYS | A | 565 | 19.982 | 47.355 | 71.392 | 1.00 | 35.75 |
| 45 | ATOM | 4514 | CE  | LYS | A | 565 | 20.796 | 46.153 | 71.842 | 1.00 | 36.31 |
|    | ATOM | 4515 | NZ  | LYS | A | 565 | 22.233 | 46.311 | 71.577 | 1.00 | 44.91 |
|    | ATOM | 4516 | N   | PHE | A | 566 | 17.321 | 51.321 | 73.073 | 1.00 | 22.91 |
|    | ATOM | 4517 | CA  | PHE | A | 566 | 17.866 | 52.423 | 73.833 | 1.00 | 24.36 |
|    | ATOM | 4518 | C   | PHE | A | 566 | 16.814 | 53.253 | 74.571 | 1.00 | 30.37 |
| 50 | ATOM | 4519 | O   | PHE | A | 566 | 16.882 | 53.540 | 75.758 | 1.00 | 30.52 |
|    | ATOM | 4520 | CB  | PHE | A | 566 | 18.622 | 53.355 | 72.857 | 1.00 | 25.26 |
|    | ATOM | 4521 | CG  | PHE | A | 566 | 19.738 | 52.677 | 72.088 | 1.00 | 24.09 |
|    | ATOM | 4522 | CD1 | PHE | A | 566 | 20.392 | 51.559 | 72.609 | 1.00 | 23.51 |
|    | ATOM | 4523 | CD2 | PHE | A | 566 | 20.165 | 53.187 | 70.858 | 1.00 | 24.48 |
| 55 | ATOM | 4524 | CE1 | PHE | A | 566 | 21.432 | 50.958 | 71.900 | 1.00 | 23.73 |
|    | ATOM | 4525 | CE2 | PHE | A | 566 | 21.211 | 52.620 | 70.129 | 1.00 | 24.75 |
|    | ATOM | 4526 | CZ  | PHE | A | 566 | 21.828 | 51.491 | 70.668 | 1.00 | 25.20 |
|    | ATOM | 4527 | N   | THR | A | 567 | 15.860 | 53.679 | 73.801 | 1.00 | 31.17 |
|    | ATOM | 4528 | CA  | THR | A | 567 | 14.783 | 54.533 | 74.239 | 1.00 | 31.74 |
| 60 | ATOM | 4529 | C   | THR | A | 567 | 13.985 | 54.037 | 75.458 | 1.00 | 33.79 |
|    | ATOM | 4530 | O   | THR | A | 567 | 13.657 | 54.818 | 76.373 | 1.00 | 26.01 |
|    | ATOM | 4531 | CB  | THR | A | 567 | 13.895 | 54.892 | 73.017 | 1.00 | 36.51 |
|    | ATOM | 4532 | OG1 | THR | A | 567 | 14.527 | 55.844 | 72.138 | 1.00 | 24.12 |
|    | ATOM | 4533 | CG2 | THR | A | 567 | 12.522 | 55.361 | 73.473 | 1.00 | 34.94 |
|    | ATOM | 4534 | N   | ARG | A | 568 | 13.663 | 52.726 | 75.469 | 1.00 | 30.74 |



|    |      |      |     |           |        |        |        |      |       |
|----|------|------|-----|-----------|--------|--------|--------|------|-------|
|    | ATOM | 4535 | CA  | ARG A 568 | 12.864 | 52.166 | 76.545 | 1.00 | 26.30 |
|    | ATOM | 4536 | C   | ARG A 568 | 13.486 | 52.226 | 77.882 | 1.00 | 28.61 |
|    | ATOM | 4537 | O   | ARG A 568 | 12.876 | 52.667 | 78.832 | 1.00 | 30.84 |
| 5  | ATOM | 4538 | CB  | ARG A 568 | 12.315 | 50.798 | 76.251 | 1.00 | 18.11 |
|    | ATOM | 4539 | CG  | ARG A 568 | 11.342 | 50.919 | 75.088 | 1.00 | 29.19 |
|    | ATOM | 4540 | CD  | ARG A 568 | 10.550 | 49.660 | 74.799 | 1.00 | 19.19 |
|    | ATOM | 4541 | NE  | ARG A 568 | 9.707  | 49.343 | 75.917 | 1.00 | 28.72 |
|    | ATOM | 4542 | CZ  | ARG A 568 | 9.254  | 48.138 | 76.133 | 1.00 | 32.39 |
| 10 | ATOM | 4543 | NH1 | ARG A 568 | 9.528  | 47.144 | 75.291 | 1.00 | 29.79 |
|    | ATOM | 4544 | NH2 | ARG A 568 | 8.507  | 47.930 | 77.208 | 1.00 | 16.44 |
|    | ATOM | 4545 | N   | PRO A 569 | 14.705 | 51.774 | 77.925 | 1.00 | 28.41 |
|    | ATOM | 4546 | CA  | PRO A 569 | 15.447 | 51.709 | 79.154 | 1.00 | 28.01 |
|    | ATOM | 4547 | C   | PRO A 569 | 15.890 | 53.042 | 79.663 | 1.00 | 32.18 |
| 15 | ATOM | 4548 | O   | PRO A 569 | 15.974 | 53.256 | 80.869 | 1.00 | 29.25 |
|    | ATOM | 4549 | CB  | PRO A 569 | 16.607 | 50.732 | 78.919 | 1.00 | 28.83 |
|    | ATOM | 4550 | CG  | PRO A 569 | 16.330 | 50.034 | 77.592 | 1.00 | 32.42 |
|    | ATOM | 4551 | CD  | PRO A 569 | 15.234 | 50.829 | 76.893 | 1.00 | 29.82 |
|    | ATOM | 4552 | N   | LEU A 570 | 16.143 | 53.949 | 78.741 | 1.00 | 31.95 |
| 20 | ATOM | 4553 | CA  | LEU A 570 | 16.560 | 55.270 | 79.160 | 1.00 | 35.11 |
|    | ATOM | 4554 | C   | LEU A 570 | 15.407 | 55.962 | 79.897 | 1.00 | 36.24 |
|    | ATOM | 4555 | O   | LEU A 570 | 15.532 | 56.506 | 81.028 | 1.00 | 34.02 |
|    | ATOM | 4556 | CB  | LEU A 570 | 17.021 | 56.110 | 77.932 | 1.00 | 37.06 |
|    | ATOM | 4557 | CG  | LEU A 570 | 18.387 | 55.701 | 77.343 | 1.00 | 41.39 |
| 25 | ATOM | 4558 | CD1 | LEU A 570 | 18.678 | 56.462 | 76.050 | 1.00 | 41.06 |
|    | ATOM | 4559 | CD2 | LEU A 570 | 19.497 | 55.984 | 78.353 | 1.00 | 37.42 |
|    | ATOM | 4560 | N   | PHE A 571 | 14.262 | 55.944 | 79.211 | 1.00 | 30.06 |
|    | ATOM | 4561 | CA  | PHE A 571 | 13.084 | 56.541 | 79.758 | 1.00 | 27.27 |
|    | ATOM | 4562 | C   | PHE A 571 | 12.813 | 55.899 | 81.095 | 1.00 | 25.94 |
| 30 | ATOM | 4563 | O   | PHE A 571 | 12.399 | 56.536 | 82.030 | 1.00 | 27.16 |
|    | ATOM | 4564 | CB  | PHE A 571 | 11.888 | 56.375 | 78.828 | 1.00 | 27.60 |
|    | ATOM | 4565 | CG  | PHE A 571 | 11.546 | 57.616 | 78.042 | 1.00 | 27.70 |
|    | ATOM | 4566 | CD1 | PHE A 571 | 11.193 | 58.820 | 78.651 | 1.00 | 29.97 |
|    | ATOM | 4567 | CD2 | PHE A 571 | 11.557 | 57.570 | 76.651 | 1.00 | 28.87 |
| 35 | ATOM | 4568 | CE1 | PHE A 571 | 10.861 | 59.953 | 77.910 | 1.00 | 28.24 |
|    | ATOM | 4569 | CE2 | PHE A 571 | 11.233 | 58.684 | 75.886 | 1.00 | 30.43 |
|    | ATOM | 4570 | CZ  | PHE A 571 | 10.877 | 59.875 | 76.520 | 1.00 | 29.55 |
|    | ATOM | 4571 | N   | LYS A 572 | 13.089 | 54.618 | 81.196 | 1.00 | 22.77 |
|    | ATOM | 4572 | CA  | LYS A 572 | 12.845 | 53.946 | 82.468 | 1.00 | 25.43 |
| 40 | ATOM | 4573 | C   | LYS A 572 | 13.783 | 54.425 | 83.561 | 1.00 | 34.48 |
|    | ATOM | 4574 | O   | LYS A 572 | 13.351 | 54.920 | 84.602 | 1.00 | 35.11 |
|    | ATOM | 4575 | CB  | LYS A 572 | 12.736 | 52.428 | 82.392 | 1.00 | 26.89 |
|    | ATOM | 4576 | CG  | LYS A 572 | 11.303 | 51.911 | 82.326 | 1.00 | 44.03 |
|    | ATOM | 4577 | CD  | LYS A 572 | 11.219 | 50.426 | 81.922 | 1.00 | 57.87 |
| 45 | ATOM | 4578 | CE  | LYS A 572 | 10.975 | 50.204 | 80.422 | 1.00 | 65.25 |
|    | ATOM | 4579 | NZ  | LYS A 572 | 11.535 | 48.954 | 79.850 | 1.00 | 61.06 |
|    | ATOM | 4580 | N   | ASP A 573 | 15.074 | 54.292 | 83.319 | 1.00 | 31.94 |
|    | ATOM | 4581 | CA  | ASP A 573 | 16.032 | 54.751 | 84.291 | 1.00 | 30.55 |
|    | ATOM | 4582 | C   | ASP A 573 | 15.684 | 56.166 | 84.712 | 1.00 | 32.26 |
| 50 | ATOM | 4583 | O   | ASP A 573 | 15.693 | 56.453 | 85.895 | 1.00 | 31.85 |
|    | ATOM | 4584 | CB  | ASP A 573 | 17.453 | 54.788 | 83.718 | 1.00 | 32.87 |
|    | ATOM | 4585 | CG  | ASP A 573 | 18.051 | 53.443 | 83.487 | 1.00 | 33.43 |
|    | ATOM | 4586 | OD1 | ASP A 573 | 17.517 | 52.422 | 83.853 | 1.00 | 29.11 |
|    | ATOM | 4587 | OD2 | ASP A 573 | 19.206 | 53.501 | 82.864 | 1.00 | 35.22 |
| 55 | ATOM | 4588 | N   | LEU A 574 | 15.387 | 57.071 | 83.745 | 1.00 | 29.50 |
|    | ATOM | 4589 | CA  | LEU A 574 | 15.062 | 58.461 | 84.109 | 1.00 | 27.65 |
|    | ATOM | 4590 | C   | LEU A 574 | 13.887 | 58.577 | 85.075 | 1.00 | 32.88 |
|    | ATOM | 4591 | O   | LEU A 574 | 13.864 | 59.411 | 85.962 | 1.00 | 31.04 |
|    | ATOM | 4592 | CB  | LEU A 574 | 14.844 | 59.385 | 82.909 | 1.00 | 26.24 |
| 60 | ATOM | 4593 | CG  | LEU A 574 | 16.068 | 59.567 | 82.027 | 1.00 | 30.41 |
|    | ATOM | 4594 | CD1 | LEU A 574 | 15.644 | 59.922 | 80.582 | 1.00 | 28.47 |
|    | ATOM | 4595 | CD2 | LEU A 574 | 16.974 | 60.659 | 82.604 | 1.00 | 27.06 |
|    | ATOM | 4596 | N   | ALA A 575 | 12.895 | 57.723 | 84.874 | 1.00 | 32.80 |
|    | ATOM | 4597 | CA  | ALA A 575 | 11.709 | 57.713 | 85.711 | 1.00 | 31.11 |
|    | ATOM | 4598 | C   | ALA A 575 | 12.002 | 57.140 | 87.083 | 1.00 | 35.71 |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
|    | ATOM | 4599 | O   | ALA | A | 575 | 11.309 | 57.362 | 88.055 | 1.00 | 39.91 |
|    | ATOM | 4600 | CB  | ALA | A | 575 | 10.631 | 56.890 | 85.024 | 1.00 | 30.56 |
|    | ATOM | 4601 | N   | ALA | A | 576 | 13.049 | 56.364 | 87.170 | 1.00 | 28.55 |
| 5  | ATOM | 4602 | CA  | ALA | A | 576 | 13.390 | 55.778 | 88.448 | 1.00 | 22.80 |
|    | ATOM | 4603 | C   | ALA | A | 576 | 14.258 | 56.724 | 89.266 | 1.00 | 26.93 |
|    | ATOM | 4604 | O   | ALA | A | 576 | 14.444 | 56.591 | 90.461 | 1.00 | 30.45 |
|    | ATOM | 4605 | CB  | ALA | A | 576 | 14.023 | 54.415 | 88.245 | 1.00 | 20.31 |
|    | ATOM | 4606 | N   | PHE | A | 577 | 14.787 | 57.686 | 88.584 | 1.00 | 22.86 |
| 10 | ATOM | 4607 | CA  | PHE | A | 577 | 15.604 | 58.673 | 89.194 | 1.00 | 22.71 |
|    | ATOM | 4608 | C   | PHE | A | 577 | 14.651 | 59.751 | 89.673 | 1.00 | 32.25 |
|    | ATOM | 4609 | O   | PHE | A | 577 | 13.930 | 60.334 | 88.863 | 1.00 | 34.17 |
|    | ATOM | 4610 | CB  | PHE | A | 577 | 16.640 | 59.188 | 88.154 | 1.00 | 22.89 |
|    | ATOM | 4611 | CG  | PHE | A | 577 | 17.704 | 60.076 | 88.741 | 1.00 | 23.16 |
| 15 | ATOM | 4612 | CD1 | PHE | A | 577 | 17.847 | 60.231 | 90.120 | 1.00 | 26.60 |
|    | ATOM | 4613 | CD2 | PHE | A | 577 | 18.561 | 60.806 | 87.914 | 1.00 | 23.46 |
|    | ATOM | 4614 | CE1 | PHE | A | 577 | 18.818 | 61.082 | 90.661 | 1.00 | 27.55 |
|    | ATOM | 4615 | CE2 | PHE | A | 577 | 19.543 | 61.657 | 88.431 | 1.00 | 23.88 |
|    | ATOM | 4616 | CZ  | PHE | A | 577 | 19.669 | 61.791 | 89.813 | 1.00 | 23.59 |
| 20 | ATOM | 4617 | N   | ASP | A | 578 | 14.625 | 60.008 | 90.990 | 1.00 | 29.70 |
|    | ATOM | 4618 | CA  | ASP | A | 578 | 13.717 | 61.018 | 91.533 | 1.00 | 28.65 |
|    | ATOM | 4619 | C   | ASP | A | 578 | 13.862 | 62.357 | 90.881 | 1.00 | 28.55 |
|    | ATOM | 4620 | O   | ASP | A | 578 | 12.877 | 63.004 | 90.599 | 1.00 | 32.65 |
|    | ATOM | 4621 | CB  | ASP | A | 578 | 13.804 | 61.192 | 93.055 | 1.00 | 32.60 |
| 25 | ATOM | 4622 | CG  | ASP | A | 578 | 15.153 | 61.647 | 93.550 | 1.00 | 53.21 |
|    | ATOM | 4623 | OD1 | ASP | A | 578 | 16.175 | 61.594 | 92.872 | 1.00 | 51.81 |
|    | ATOM | 4624 | OD2 | ASP | A | 578 | 15.104 | 62.072 | 94.796 | 1.00 | 64.93 |
|    | ATOM | 4625 | N   | LYS | A | 579 | 15.104 | 62.750 | 90.674 | 1.00 | 20.12 |
|    | ATOM | 4626 | CA  | LYS | A | 579 | 15.470 | 64.012 | 90.084 | 1.00 | 21.01 |
| 30 | ATOM | 4627 | C   | LYS | A | 579 | 14.934 | 64.270 | 88.697 | 1.00 | 30.25 |
|    | ATOM | 4628 | O   | LYS | A | 579 | 14.620 | 65.413 | 88.368 | 1.00 | 35.12 |
|    | ATOM | 4629 | CB  | LYS | A | 579 | 16.982 | 64.223 | 90.104 | 1.00 | 24.11 |
|    | ATOM | 4630 | CG  | LYS | A | 579 | 17.552 | 64.202 | 91.512 | 1.00 | 48.98 |
|    | ATOM | 4631 | CD  | LYS | A | 579 | 17.252 | 65.488 | 92.286 | 1.00 | 76.92 |
| 35 | ATOM | 4632 | CE  | LYS | A | 579 | 16.495 | 65.258 | 93.588 | 1.00 | 87.93 |
|    | ATOM | 4633 | NZ  | LYS | A | 579 | 17.282 | 64.550 | 94.611 | 1.00 | 89.56 |
|    | ATOM | 4634 | N   | SER | A | 580 | 14.838 | 63.244 | 87.857 | 1.00 | 28.66 |
|    | ATOM | 4635 | CA  | SER | A | 580 | 14.368 | 63.437 | 86.459 | 1.00 | 28.56 |
|    | ATOM | 4636 | C   | SER | A | 580 | 13.007 | 62.829 | 86.129 | 1.00 | 32.95 |
| 40 | ATOM | 4637 | O   | SER | A | 580 | 12.561 | 62.870 | 84.992 | 1.00 | 35.30 |
|    | ATOM | 4638 | CB  | SER | A | 580 | 15.337 | 62.774 | 85.517 | 1.00 | 25.69 |
|    | ATOM | 4639 | OG  | SER | A | 580 | 15.476 | 61.424 | 85.969 | 1.00 | 25.12 |
|    | ATOM | 4640 | N   | HIS | A | 581 | 12.364 | 62.230 | 87.098 | 1.00 | 26.81 |
| 45 | ATOM | 4641 | CA  | HIS | A | 581 | 11.100 | 61.595 | 86.850 | 1.00 | 28.26 |
|    | ATOM | 4642 | C   | HIS | A | 581 | 10.067 | 62.399 | 86.042 | 1.00 | 36.50 |
|    | ATOM | 4643 | O   | HIS | A | 581 | 9.644  | 62.031 | 84.927 | 1.00 | 34.71 |
|    | ATOM | 4644 | CB  | HIS | A | 581 | 10.553 | 61.047 | 88.152 | 1.00 | 29.76 |
|    | ATOM | 4645 | CG  | HIS | A | 581 | 9.148  | 60.588 | 87.968 | 1.00 | 35.31 |
|    | ATOM | 4646 | ND1 | HIS | A | 581 | 8.111  | 61.494 | 87.899 | 1.00 | 38.92 |
| 50 | ATOM | 4647 | CD2 | HIS | A | 581 | 8.634  | 59.338 | 87.891 | 1.00 | 36.84 |
|    | ATOM | 4648 | CE1 | HIS | A | 581 | 6.999  | 60.783 | 87.817 | 1.00 | 38.85 |
|    | ATOM | 4649 | NE2 | HIS | A | 581 | 7.280  | 59.488 | 87.734 | 1.00 | 38.13 |
|    | ATOM | 4650 | N   | ASP | A | 582 | 9.656  | 63.502 | 86.639 | 1.00 | 35.79 |
|    | ATOM | 4651 | CA  | ASP | A | 582 | 8.680  | 64.388 | 86.064 | 1.00 | 34.39 |
| 55 | ATOM | 4652 | C   | ASP | A | 582 | 9.035  | 64.807 | 84.659 | 1.00 | 37.82 |
|    | ATOM | 4653 | O   | ASP | A | 582 | 8.220  | 64.704 | 83.735 | 1.00 | 37.01 |
|    | ATOM | 4654 | CB  | ASP | A | 582 | 8.428  | 65.552 | 87.001 | 1.00 | 36.57 |
|    | ATOM | 4655 | CG  | ASP | A | 582 | 7.597  | 65.110 | 88.167 | 1.00 | 58.09 |
|    | ATOM | 4656 | OD1 | ASP | A | 582 | 6.708  | 64.289 | 88.070 | 1.00 | 63.17 |
| 60 | ATOM | 4657 | OD2 | ASP | A | 582 | 7.920  | 65.708 | 89.279 | 1.00 | 73.96 |
|    | ATOM | 4658 | N   | GLN | A | 583 | 10.272 | 65.255 | 84.488 | 1.00 | 32.88 |
|    | ATOM | 4659 | CA  | GLN | A | 583 | 10.750 | 65.648 | 83.169 | 1.00 | 29.92 |
|    | ATOM | 4660 | C   | GLN | A | 583 | 10.690 | 64.464 | 82.168 | 1.00 | 37.12 |
|    | ATOM | 4661 | O   | GLN | A | 583 | 10.362 | 64.624 | 80.990 | 1.00 | 37.42 |
|    | ATOM | 4662 | CB  | GLN | A | 583 | 12.172 | 66.182 | 83.287 | 1.00 | 28.54 |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
|    | ATOM | 4663 | CG  | GLN | A | 583 | 12.704 | 66.648 | 81.929 | 1.00 | 48.12 |
|    | ATOM | 4664 | CD  | GLN | A | 583 | 13.957 | 67.475 | 82.081 | 1.00 | 64.09 |
|    | ATOM | 4665 | OE1 | GLN | A | 583 | 14.736 | 67.248 | 83.015 | 1.00 | 59.43 |
| 5  | ATOM | 4666 | NE2 | GLN | A | 583 | 14.130 | 68.461 | 81.201 | 1.00 | 55.34 |
|    | ATOM | 4667 | N   | ALA | A | 584 | 11.009 | 63.250 | 82.638 | 1.00 | 33.22 |
|    | ATOM | 4668 | CA  | ALA | A | 584 | 10.964 | 62.062 | 81.780 | 1.00 | 32.22 |
|    | ATOM | 4669 | C   | ALA | A | 584 | 9.557  | 61.841 | 81.315 | 1.00 | 37.45 |
|    | ATOM | 4670 | O   | ALA | A | 584 | 9.319  | 61.526 | 80.152 | 1.00 | 40.05 |
| 10 | ATOM | 4671 | CB  | ALA | A | 584 | 11.389 | 60.793 | 82.504 | 1.00 | 31.62 |
|    | ATOM | 4672 | N   | VAL | A | 585 | 8.622  | 61.995 | 82.261 | 1.00 | 30.42 |
|    | ATOM | 4673 | CA  | VAL | A | 585 | 7.217  | 61.806 | 81.946 | 1.00 | 29.16 |
|    | ATOM | 4674 | C   | VAL | A | 585 | 6.647  | 62.909 | 81.024 | 1.00 | 36.53 |
|    | ATOM | 4675 | O   | VAL | A | 585 | 5.933  | 62.690 | 80.052 | 1.00 | 36.22 |
| 15 | ATOM | 4676 | CB  | VAL | A | 585 | 6.408  | 61.567 | 83.209 | 1.00 | 29.78 |
|    | ATOM | 4677 | CG1 | VAL | A | 585 | 4.959  | 61.947 | 82.955 | 1.00 | 30.03 |
|    | ATOM | 4678 | CG2 | VAL | A | 585 | 6.464  | 60.085 | 83.539 | 1.00 | 27.82 |
|    | ATOM | 4679 | N   | ARG | A | 586 | 7.000  | 64.123 | 81.333 | 1.00 | 35.76 |
|    | ATOM | 4680 | CA  | ARG | A | 586 | 6.574  | 65.242 | 80.562 | 1.00 | 36.20 |
| 20 | ATOM | 4681 | C   | ARG | A | 586 | 7.146  | 65.125 | 79.180 | 1.00 | 44.65 |
|    | ATOM | 4682 | O   | ARG | A | 586 | 6.459  | 65.355 | 78.197 | 1.00 | 48.32 |
|    | ATOM | 4683 | CB  | ARG | A | 586 | 7.116  | 66.498 | 81.208 | 1.00 | 38.13 |
|    | ATOM | 4684 | CG  | ARG | A | 586 | 6.744  | 67.799 | 80.518 | 1.00 | 61.01 |
|    | ATOM | 4685 | CD  | ARG | A | 586 | 7.077  | 69.029 | 81.354 | 1.00 | 73.03 |
| 25 | ATOM | 4686 | NE  | ARG | A | 586 | 8.491  | 69.128 | 81.711 | 1.00 | 86.05 |
|    | ATOM | 4687 | CZ  | ARG | A | 586 | 8.961  | 69.001 | 82.957 | 1.00 | 98.46 |
|    | ATOM | 4688 | NH1 | ARG | A | 586 | 8.167  | 68.741 | 84.004 | 1.00 | 79.75 |
|    | ATOM | 4689 | NH2 | ARG | A | 586 | 10.268 | 69.103 | 83.159 | 1.00 | 77.55 |
|    | ATOM | 4690 | N   | THR | A | 587 | 8.426  | 64.769 | 79.110 | 1.00 | 39.49 |
| 30 | ATOM | 4691 | CA  | THR | A | 587 | 9.099  | 64.646 | 77.822 | 1.00 | 36.80 |
|    | ATOM | 4692 | C   | THR | A | 587 | 8.387  | 63.690 | 76.869 | 1.00 | 37.11 |
|    | ATOM | 4693 | O   | THR | A | 587 | 8.229  | 63.931 | 75.678 | 1.00 | 36.91 |
|    | ATOM | 4694 | CB  | THR | A | 587 | 10.634 | 64.384 | 77.917 | 1.00 | 39.40 |
|    | ATOM | 4695 | OG1 | THR | A | 587 | 11.303 | 65.334 | 78.717 | 1.00 | 46.27 |
| 35 | ATOM | 4696 | CG2 | THR | A | 587 | 11.233 | 64.460 | 76.529 | 1.00 | 32.60 |
|    | ATOM | 4697 | N   | TYR | A | 588 | 7.934  | 62.587 | 77.393 | 1.00 | 33.33 |
|    | ATOM | 4698 | CA  | TYR | A | 588 | 7.252  | 61.639 | 76.555 | 1.00 | 33.94 |
|    | ATOM | 4699 | C   | TYR | A | 588 | 5.890  | 62.146 | 76.090 | 1.00 | 37.02 |
|    | ATOM | 4700 | O   | TYR | A | 588 | 5.428  | 61.880 | 74.988 | 1.00 | 41.55 |
| 40 | ATOM | 4701 | CB  | TYR | A | 588 | 7.042  | 60.383 | 77.396 | 1.00 | 33.96 |
|    | ATOM | 4702 | CG  | TYR | A | 588 | 6.017  | 59.440 | 76.851 | 1.00 | 33.08 |
|    | ATOM | 4703 | CD1 | TYR | A | 588 | 6.331  | 58.640 | 75.754 | 1.00 | 35.64 |
|    | ATOM | 4704 | CD2 | TYR | A | 588 | 4.758  | 59.288 | 77.437 | 1.00 | 34.09 |
|    | ATOM | 4705 | CE1 | TYR | A | 588 | 5.424  | 57.703 | 75.251 | 1.00 | 34.36 |
| 45 | ATOM | 4706 | CE2 | TYR | A | 588 | 3.822  | 58.378 | 76.932 | 1.00 | 34.05 |
|    | ATOM | 4707 | CZ  | TYR | A | 588 | 4.162  | 57.581 | 75.834 | 1.00 | 33.89 |
|    | ATOM | 4708 | OH  | TYR | A | 588 | 3.275  | 56.674 | 75.322 | 1.00 | 23.43 |
|    | ATOM | 4709 | N   | GLN | A | 589 | 5.216  | 62.853 | 76.959 | 1.00 | 25.04 |
|    | ATOM | 4710 | CA  | GLN | A | 589 | 3.914  | 63.339 | 76.612 | 1.00 | 21.41 |
| 50 | ATOM | 4711 | C   | GLN | A | 589 | 3.992  | 64.304 | 75.481 | 1.00 | 28.78 |
|    | ATOM | 4712 | O   | GLN | A | 589 | 3.099  | 64.410 | 74.678 | 1.00 | 31.24 |
|    | ATOM | 4713 | CB  | GLN | A | 589 | 3.241  | 63.935 | 77.832 | 1.00 | 21.73 |
|    | ATOM | 4714 | CG  | GLN | A | 589 | 2.878  | 62.820 | 78.827 | 1.00 | 22.30 |
|    | ATOM | 4715 | CD  | GLN | A | 589 | 1.695  | 62.069 | 78.293 | 1.00 | 52.83 |
| 55 | ATOM | 4716 | OE1 | GLN | A | 589 | 1.511  | 62.003 | 77.075 | 1.00 | 60.15 |
|    | ATOM | 4717 | NE2 | GLN | A | 589 | 0.864  | 61.542 | 79.182 | 1.00 | 53.04 |
|    | ATOM | 4718 | N   | GLU | A | 590 | 5.099  | 65.001 | 75.409 | 1.00 | 28.36 |
|    | ATOM | 4719 | CA  | GLU | A | 590 | 5.276  | 65.966 | 74.355 | 1.00 | 26.87 |
|    | ATOM | 4720 | C   | GLU | A | 590 | 5.840  | 65.338 | 73.140 | 1.00 | 35.10 |
| 60 | ATOM | 4721 | O   | GLU | A | 590 | 6.096  | 66.059 | 72.171 | 1.00 | 40.28 |
|    | ATOM | 4722 | CB  | GLU | A | 590 | 6.323  | 67.011 | 74.747 | 1.00 | 27.61 |
|    | ATOM | 4723 | CG  | GLU | A | 590 | 5.846  | 67.954 | 75.847 | 1.00 | 44.11 |
|    | ATOM | 4724 | CD  | GLU | A | 590 | 6.981  | 68.759 | 76.388 | 1.00 | 75.35 |
|    | ATOM | 4725 | OE1 | GLU | A | 590 | 8.120  | 68.689 | 75.925 | 1.00 | 54.78 |
|    | ATOM | 4726 | OE2 | GLU | A | 590 | 6.609  | 69.516 | 77.403 | 1.00 | 59.46 |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| 5  | ATOM | 4727 | N   | HIS | A | 591 | 6.091  | 64.031 | 73.207 | 1.00 | 27.57 |
|    | ATOM | 4728 | CA  | HIS | A | 591 | 6.713  | 63.384 | 72.086 | 1.00 | 25.58 |
|    | ATOM | 4729 | C   | HIS | A | 591 | 5.928  | 62.249 | 71.578 | 1.00 | 32.34 |
|    | ATOM | 4730 | O   | HIS | A | 591 | 6.184  | 61.751 | 70.496 | 1.00 | 38.53 |
|    | ATOM | 4731 | CB  | HIS | A | 591 | 8.094  | 62.851 | 72.487 | 1.00 | 26.32 |
| 10 | ATOM | 4732 | CG  | HIS | A | 591 | 9.219  | 63.809 | 72.268 | 1.00 | 31.06 |
|    | ATOM | 4733 | ND1 | HIS | A | 591 | 9.630  | 64.680 | 73.255 | 1.00 | 32.65 |
|    | ATOM | 4734 | CD2 | HIS | A | 591 | 9.998  | 64.032 | 71.169 | 1.00 | 34.91 |
|    | ATOM | 4735 | CE1 | HIS | A | 591 | 10.635 | 65.404 | 72.756 | 1.00 | 32.01 |
|    | ATOM | 4736 | NE2 | HIS | A | 591 | 10.884 | 65.037 | 71.508 | 1.00 | 33.36 |
| 15 | ATOM | 4737 | N   | LYS | A | 592 | 4.978  | 61.812 | 72.337 | 1.00 | 28.34 |
|    | ATOM | 4738 | CA  | LYS | A | 592 | 4.254  | 60.643 | 71.849 | 1.00 | 29.96 |
|    | ATOM | 4739 | C   | LYS | A | 592 | 3.654  | 60.692 | 70.432 | 1.00 | 33.41 |
|    | ATOM | 4740 | O   | LYS | A | 592 | 3.819  | 59.769 | 69.592 | 1.00 | 29.05 |
|    | ATOM | 4741 | CB  | LYS | A | 592 | 3.362  | 59.983 | 72.888 | 1.00 | 32.83 |
| 20 | ATOM | 4742 | CG  | LYS | A | 592 | 2.435  | 60.930 | 73.615 | 1.00 | 31.14 |
|    | ATOM | 4743 | CD  | LYS | A | 592 | 1.677  | 60.203 | 74.704 | 1.00 | 38.97 |
|    | ATOM | 4744 | CE  | LYS | A | 592 | 0.253  | 60.691 | 74.890 | 1.00 | 25.02 |
|    | ATOM | 4745 | NZ  | LYS | A | 592 | -0.157 | 60.632 | 76.302 | 1.00 | 45.83 |
|    | ATOM | 4746 | N   | ALA | A | 593 | 2.934  | 61.782 | 70.187 | 1.00 | 30.97 |
| 25 | ATOM | 4747 | CA  | ALA | A | 593 | 2.260  | 62.026 | 68.917 | 1.00 | 28.47 |
|    | ATOM | 4748 | C   | ALA | A | 593 | 3.169  | 61.943 | 67.703 | 1.00 | 32.66 |
|    | ATOM | 4749 | O   | ALA | A | 593 | 2.775  | 61.488 | 66.639 | 1.00 | 36.77 |
|    | ATOM | 4750 | CB  | ALA | A | 593 | 1.571  | 63.379 | 68.954 | 1.00 | 27.35 |
|    | ATOM | 4751 | N   | SER | A | 594 | 4.384  | 62.405 | 67.869 | 1.00 | 27.08 |
| 30 | ATOM | 4752 | CA  | SER | A | 594 | 5.345  | 62.417 | 66.794 | 1.00 | 30.04 |
|    | ATOM | 4753 | C   | SER | A | 594 | 6.185  | 61.169 | 66.760 | 1.00 | 36.80 |
|    | ATOM | 4754 | O   | SER | A | 594 | 6.995  | 60.991 | 65.848 | 1.00 | 37.94 |
|    | ATOM | 4755 | CB  | SER | A | 594 | 6.292  | 63.596 | 66.977 | 1.00 | 37.69 |
|    | ATOM | 4756 | OG  | SER | A | 594 | 7.199  | 63.340 | 68.043 | 1.00 | 54.55 |
| 35 | ATOM | 4757 | N   | MET | A | 595 | 6.015  | 60.340 | 67.776 | 1.00 | 33.12 |
|    | ATOM | 4758 | CA  | MET | A | 595 | 6.794  | 59.115 | 67.898 | 1.00 | 33.96 |
|    | ATOM | 4759 | C   | MET | A | 595 | 6.200  | 57.936 | 67.125 | 1.00 | 40.91 |
|    | ATOM | 4760 | O   | MET | A | 595 | 5.019  | 57.927 | 66.809 | 1.00 | 50.82 |
|    | ATOM | 4761 | CB  | MET | A | 595 | 6.716  | 58.686 | 69.382 | 1.00 | 34.22 |
| 40 | ATOM | 4762 | CG  | MET | A | 595 | 7.621  | 59.371 | 70.399 | 1.00 | 34.61 |
|    | ATOM | 4763 | SD  | MET | A | 595 | 7.606  | 58.440 | 71.962 | 1.00 | 39.24 |
|    | ATOM | 4764 | CE  | MET | A | 595 | 7.145  | 59.779 | 73.084 | 1.00 | 36.72 |
|    | ATOM | 4765 | N   | HIS | A | 596 | 6.987  | 56.897 | 66.886 | 1.00 | 26.19 |
|    | ATOM | 4766 | CA  | HIS | A | 596 | 6.496  | 55.657 | 66.246 | 1.00 | 23.19 |
| 45 | ATOM | 4767 | C   | HIS | A | 596 | 5.438  | 54.964 | 67.120 | 1.00 | 25.21 |
|    | ATOM | 4768 | O   | HIS | A | 596 | 5.621  | 54.728 | 68.311 | 1.00 | 22.59 |
|    | ATOM | 4769 | CB  | HIS | A | 596 | 7.657  | 54.655 | 66.077 | 1.00 | 24.41 |
|    | ATOM | 4770 | CG  | HIS | A | 596 | 7.222  | 53.366 | 65.493 | 1.00 | 30.13 |
|    | ATOM | 4771 | ND1 | HIS | A | 596 | 7.606  | 52.995 | 64.214 | 1.00 | 32.86 |
| 50 | ATOM | 4772 | CD2 | HIS | A | 596 | 6.421  | 52.385 | 66.005 | 1.00 | 30.90 |
|    | ATOM | 4773 | CE1 | HIS | A | 596 | 7.047  | 51.824 | 63.974 | 1.00 | 30.05 |
|    | ATOM | 4774 | NE2 | HIS | A | 596 | 6.325  | 51.441 | 65.031 | 1.00 | 30.20 |
|    | ATOM | 4775 | N   | PRO | A | 597 | 4.334  | 54.587 | 66.512 | 1.00 | 27.08 |
|    | ATOM | 4776 | CA  | PRO | A | 597 | 3.217  | 53.912 | 67.173 | 1.00 | 26.35 |
| 55 | ATOM | 4777 | C   | PRO | A | 597 | 3.513  | 52.851 | 68.248 | 1.00 | 37.51 |
|    | ATOM | 4778 | O   | PRO | A | 597 | 2.979  | 52.900 | 69.348 | 1.00 | 41.16 |
|    | ATOM | 4779 | CB  | PRO | A | 597 | 2.334  | 53.307 | 66.076 | 1.00 | 26.17 |
|    | ATOM | 4780 | CG  | PRO | A | 597 | 3.140  | 53.426 | 64.792 | 1.00 | 34.56 |
|    | ATOM | 4781 | CD  | PRO | A | 597 | 4.285  | 54.418 | 65.050 | 1.00 | 30.06 |
| 60 | ATOM | 4782 | N   | VAL | A | 598 | 4.311  | 51.850 | 67.939 | 1.00 | 33.08 |
|    | ATOM | 4783 | CA  | VAL | A | 598 | 4.585  | 50.802 | 68.911 | 1.00 | 28.39 |
|    | ATOM | 4784 | C   | VAL | A | 598 | 5.444  | 51.307 | 70.029 | 1.00 | 29.32 |
|    | ATOM | 4785 | O   | VAL | A | 598 | 5.168  | 51.096 | 71.217 | 1.00 | 29.13 |
|    | ATOM | 4786 | CB  | VAL | A | 598 | 5.196  | 49.599 | 68.210 | 1.00 | 27.99 |
|    | ATOM | 4787 | CG1 | VAL | A | 598 | 5.806  | 48.608 | 69.187 | 1.00 | 26.98 |
|    | ATOM | 4788 | CG2 | VAL | A | 598 | 4.144  | 48.944 | 67.296 | 1.00 | 26.13 |
|    | ATOM | 4789 | N   | THR | A | 599 | 6.480  | 52.021 | 69.635 | 1.00 | 26.10 |
|    | ATOM | 4790 | CA  | THR | A | 599 | 7.370  | 52.573 | 70.631 | 1.00 | 26.95 |



|    |      |      |     |     |   |     |       |        |        |      |       |
|----|------|------|-----|-----|---|-----|-------|--------|--------|------|-------|
|    | ATOM | 4791 | C   | THR | A | 599 | 6.650 | 53.404 | 71.669 | 1.00 | 30.81 |
|    | ATOM | 4792 | O   | THR | A | 599 | 6.863 | 53.327 | 72.871 | 1.00 | 31.33 |
|    | ATOM | 4793 | CB  | THR | A | 599 | 8.413 | 53.455 | 69.975 | 1.00 | 26.67 |
| 5  | ATOM | 4794 | OG1 | THR | A | 599 | 9.092 | 52.725 | 68.958 | 1.00 | 27.92 |
|    | ATOM | 4795 | CG2 | THR | A | 599 | 9.358 | 53.884 | 71.092 | 1.00 | 20.69 |
|    | ATOM | 4796 | N   | ALA | A | 600 | 5.801 | 54.218 | 71.135 | 1.00 | 26.41 |
|    | ATOM | 4797 | CA  | ALA | A | 600 | 4.997 | 55.111 | 71.878 | 1.00 | 26.39 |
|    | ATOM | 4798 | C   | ALA | A | 600 | 4.176 | 54.339 | 72.860 | 1.00 | 32.00 |
| 10 | ATOM | 4799 | O   | ALA | A | 600 | 4.162 | 54.597 | 74.057 | 1.00 | 35.37 |
|    | ATOM | 4800 | CB  | ALA | A | 600 | 4.090 | 55.774 | 70.856 | 1.00 | 27.56 |
|    | ATOM | 4801 | N   | MET | A | 601 | 3.470 | 53.380 | 72.332 | 1.00 | 26.26 |
|    | ATOM | 4802 | CA  | MET | A | 601 | 2.627 | 52.585 | 73.167 | 1.00 | 26.60 |
|    | ATOM | 4803 | C   | MET | A | 601 | 3.439 | 51.909 | 74.225 | 1.00 | 25.73 |
| 15 | ATOM | 4804 | O   | MET | A | 601 | 3.099 | 51.964 | 75.381 | 1.00 | 25.77 |
|    | ATOM | 4805 | CB  | MET | A | 601 | 1.752 | 51.625 | 72.353 | 1.00 | 30.49 |
|    | ATOM | 4806 | CG  | MET | A | 601 | 1.024 | 50.594 | 73.176 | 1.00 | 36.00 |
|    | ATOM | 4807 | SD  | MET | A | 601 | 2.043 | 49.146 | 73.554 | 1.00 | 42.41 |
|    | ATOM | 4808 | CE  | MET | A | 601 | 1.693 | 48.128 | 72.111 | 1.00 | 37.75 |
| 20 | ATOM | 4809 | N   | LEU | A | 602 | 4.538 | 51.310 | 73.848 | 1.00 | 21.64 |
|    | ATOM | 4810 | CA  | LEU | A | 602 | 5.339 | 50.671 | 74.873 | 1.00 | 22.59 |
|    | ATOM | 4811 | C   | LEU | A | 602 | 6.010 | 51.650 | 75.870 | 1.00 | 29.61 |
|    | ATOM | 4812 | O   | LEU | A | 602 | 6.137 | 51.346 | 77.039 | 1.00 | 27.62 |
|    | ATOM | 4813 | CB  | LEU | A | 602 | 6.418 | 49.760 | 74.294 | 1.00 | 22.14 |
| 25 | ATOM | 4814 | CG  | LEU | A | 602 | 5.916 | 48.529 | 73.575 | 1.00 | 25.78 |
|    | ATOM | 4815 | CD1 | LEU | A | 602 | 7.021 | 48.087 | 72.609 | 1.00 | 26.02 |
|    | ATOM | 4816 | CD2 | LEU | A | 602 | 5.651 | 47.445 | 74.613 | 1.00 | 21.01 |
|    | ATOM | 4817 | N   | VAL | A | 603 | 6.508 | 52.805 | 75.445 | 1.00 | 27.15 |
|    | ATOM | 4818 | CA  | VAL | A | 603 | 7.145 | 53.684 | 76.413 | 1.00 | 26.39 |
| 30 | ATOM | 4819 | C   | VAL | A | 603 | 6.121 | 54.157 | 77.438 | 1.00 | 32.60 |
|    | ATOM | 4820 | O   | VAL | A | 603 | 6.436 | 54.235 | 78.621 | 1.00 | 35.31 |
|    | ATOM | 4821 | CB  | VAL | A | 603 | 7.917 | 54.832 | 75.760 | 1.00 | 27.78 |
|    | ATOM | 4822 | CG1 | VAL | A | 603 | 8.286 | 55.887 | 76.774 | 1.00 | 24.54 |
|    | ATOM | 4823 | CG2 | VAL | A | 603 | 9.172 | 54.286 | 75.094 | 1.00 | 27.29 |
| 35 | ATOM | 4824 | N   | GLY | A | 604 | 4.878 | 54.434 | 76.976 | 1.00 | 27.44 |
|    | ATOM | 4825 | CA  | GLY | A | 604 | 3.759 | 54.856 | 77.819 | 1.00 | 27.58 |
|    | ATOM | 4826 | C   | GLY | A | 604 | 3.418 | 53.797 | 78.905 | 1.00 | 37.00 |
|    | ATOM | 4827 | O   | GLY | A | 604 | 3.088 | 54.102 | 80.072 | 1.00 | 36.56 |
|    | ATOM | 4828 | N   | LYS | A | 605 | 3.511 | 52.522 | 78.520 | 1.00 | 32.54 |
| 40 | ATOM | 4829 | CA  | LYS | A | 605 | 3.250 | 51.415 | 79.459 | 1.00 | 32.17 |
|    | ATOM | 4830 | C   | LYS | A | 605 | 4.312 | 51.405 | 80.539 | 1.00 | 35.15 |
|    | ATOM | 4831 | O   | LYS | A | 605 | 4.040 | 51.347 | 81.734 | 1.00 | 33.77 |
|    | ATOM | 4832 | CB  | LYS | A | 605 | 3.231 | 50.034 | 78.782 | 1.00 | 33.59 |
|    | ATOM | 4833 | CG  | LYS | A | 605 | 1.837 | 49.438 | 78.576 | 1.00 | 42.45 |
| 45 | ATOM | 4834 | CD  | LYS | A | 605 | 1.846 | 48.115 | 77.815 | 1.00 | 60.83 |
|    | ATOM | 4835 | CE  | LYS | A | 605 | 1.223 | 46.946 | 78.578 | 1.00 | 86.38 |
|    | ATOM | 4836 | NZ  | LYS | A | 605 | 2.188 | 46.179 | 79.385 | 1.00 | 93.05 |
|    | ATOM | 4837 | N   | ASP | A | 606 | 5.544 | 51.470 | 80.056 | 1.00 | 32.91 |
|    | ATOM | 4838 | CA  | ASP | A | 606 | 6.715 | 51.510 | 80.878 | 1.00 | 31.82 |
| 50 | ATOM | 4839 | C   | ASP | A | 606 | 6.549 | 52.667 | 81.833 | 1.00 | 36.24 |
|    | ATOM | 4840 | O   | ASP | A | 606 | 6.652 | 52.503 | 83.045 | 1.00 | 35.19 |
|    | ATOM | 4841 | CB  | ASP | A | 606 | 7.983 | 51.702 | 80.027 | 1.00 | 32.52 |
|    | ATOM | 4842 | CG  | ASP | A | 606 | 8.302 | 50.525 | 79.134 | 1.00 | 40.01 |
|    | ATOM | 4843 | OD1 | ASP | A | 606 | 7.934 | 49.378 | 79.344 | 1.00 | 40.49 |
| 55 | ATOM | 4844 | OD2 | ASP | A | 606 | 9.038 | 50.869 | 78.111 | 1.00 | 41.73 |
|    | ATOM | 4845 | N   | LEU | A | 607 | 6.240 | 53.833 | 81.266 | 1.00 | 34.45 |
|    | ATOM | 4846 | CA  | LEU | A | 607 | 6.152 | 54.972 | 82.185 | 1.00 | 36.03 |
|    | ATOM | 4847 | C   | LEU | A | 607 | 4.814 | 55.018 | 82.968 | 1.00 | 42.35 |
|    | ATOM | 4848 | O   | LEU | A | 607 | 4.600 | 55.872 | 83.824 | 1.00 | 41.57 |
| 60 | ATOM | 4849 | CB  | LEU | A | 607 | 6.321 | 56.250 | 81.364 | 1.00 | 36.90 |
|    | ATOM | 4850 | CG  | LEU | A | 607 | 7.779 | 56.490 | 80.974 | 1.00 | 38.75 |
|    | ATOM | 4851 | CD1 | LEU | A | 607 | 7.954 | 57.746 | 80.132 | 1.00 | 34.34 |
|    | ATOM | 4852 | CD2 | LEU | A | 607 | 8.695 | 56.653 | 82.183 | 1.00 | 41.97 |
|    | ATOM | 4853 | N   | LYS | A | 608 | 3.895 | 54.062 | 82.586 | 1.00 | 45.01 |
|    | ATOM | 4854 | CA  | LYS | A | 608 | 2.576 | 53.874 | 83.264 | 1.00 | 46.99 |



|    |      |      |      |     |   |     |         |        |        |      |        |
|----|------|------|------|-----|---|-----|---------|--------|--------|------|--------|
|    | ATOM | 4855 | C    | LYS | A | 608 | 1.625   | 55.088 | 83.181 | 1.00 | 51.31  |
|    | ATOM | 4856 | O    | LYS | A | 608 | 0.988   | 55.467 | 84.151 | 1.00 | 51.35  |
|    | ATOM | 4857 | CB   | LYS | A | 608 | 2.813   | 53.510 | 84.750 | 1.00 | 50.83  |
| 5  | ATOM | 4858 | CG   | LYS | A | 608 | 3.331   | 52.093 | 84.949 | 1.00 | 63.57  |
|    | ATOM | 4859 | CD   | LYS | A | 608 | 4.405   | 52.019 | 86.031 | 1.00 | 77.03  |
|    | ATOM | 4860 | CE   | LYS | A | 608 | 5.341   | 50.825 | 85.858 | 1.00 | 96.40  |
|    | ATOM | 4861 | NZ   | LYS | A | 608 | 6.034   | 50.554 | 87.117 | 1.00 | 100.00 |
|    | ATOM | 4862 | N    | VAL | A | 609 | 1.560   | 55.724 | 81.991 | 1.00 | 50.28  |
| 10 | ATOM | 4863 | CA   | VAL | A | 609 | 0.688   | 56.901 | 81.852 | 1.00 | 50.89  |
|    | ATOM | 4864 | C    | VAL | A | 609 | -0.494  | 56.660 | 80.897 | 1.00 | 60.23  |
|    | ATOM | 4865 | O    | VAL | A | 609 | -1.640  | 56.952 | 81.194 | 1.00 | 63.02  |
|    | ATOM | 4866 | CB   | VAL | A | 609 | 1.533   | 58.091 | 81.364 | 1.00 | 54.72  |
|    | ATOM | 4867 | CG1  | VAL | A | 609 | 1.996   | 58.926 | 82.551 | 1.00 | 54.87  |
|    | ATOM | 4868 | CG2  | VAL | A | 609 | 2.744   | 57.607 | 80.605 | 1.00 | 54.46  |
| 15 | ATOM | 4869 | N    | ASP | A | 610 | -0.177  | 56.152 | 79.687 | 1.00 | 58.84  |
|    | ATOM | 4870 | CA   | ASP | A | 610 | -1.238  | 55.949 | 78.699 | 1.00 | 99.84  |
|    | ATOM | 4871 | C    | ASP | A | 610 | -2.062  | 54.695 | 79.001 | 1.00 | 100.00 |
|    | ATOM | 4872 | O    | ASP | A | 610 | -3.247  | 54.615 | 78.711 | 1.00 | 69.75  |
|    | ATOM | 4873 | CB   | ASP | A | 610 | -0.594  | 55.818 | 77.316 | 1.00 | 100.00 |
| 20 | ATOM | 4874 | CG   | ASP | A | 610 | -0.637  | 57.161 | 76.610 | 1.00 | 92.61  |
|    | ATOM | 4875 | OD1  | ASP | A | 610 | -1.449  | 57.999 | 77.018 | 1.00 | 90.49  |
|    | ATOM | 4876 | OD2  | ASP | A | 610 | 0.134   | 57.355 | 75.670 | 1.00 | 89.29  |
|    | ATOM | 4877 | ZN2+ | ZN  | Z | 1   | 17.003  | 38.803 | 64.180 | 1.00 | 28.37  |
|    | ATOM | 4878 | YB3+ | YB  | Y | 1   | 43.011  | 51.068 | 98.864 | 1.00 | 34.70  |
| 25 | ATOM | 4879 | YB3+ | YB  | Y | 2   | -13.786 | 56.771 | 52.040 | 0.50 | 57.25  |
|    | ATOM | 4880 | YB3+ | YB  | Y | 3   | -10.537 | 57.860 | 52.381 | 0.50 | 36.57  |
|    | ATOM | 4881 | CG   | IMD | I | 1   | 26.249  | 42.039 | 80.754 | 1.00 | 28.44  |
|    | ATOM | 4882 | ND1  | IMD | I | 1   | 26.057  | 42.254 | 79.400 | 1.00 | 28.35  |
|    | ATOM | 4883 | CD2  | IMD | I | 1   | 27.562  | 41.726 | 80.902 | 1.00 | 17.99  |
| 30 | ATOM | 4884 | CE1  | IMD | I | 1   | 27.201  | 42.063 | 78.760 | 1.00 | 29.77  |
|    | ATOM | 4885 | NE2  | IMD | I | 1   | 28.130  | 41.745 | 79.647 | 1.00 | 35.02  |
|    | ATOM | 4886 | CB   | ACE | C | 1   | 13.616  | 12.333 | 68.475 | 1.00 | 59.33  |
|    | ATOM | 4887 | CG   | ACE | C | 1   | 12.871  | 13.331 | 69.306 | 1.00 | 42.98  |
|    | ATOM | 4888 | OD1  | ACE | C | 1   | 12.958  | 14.536 | 69.146 | 1.00 | 39.66  |
| 35 | ATOM | 4889 | OD2  | ACE | C | 1   | 12.142  | 12.759 | 70.236 | 1.00 | 47.21  |
|    | ATOM | 4890 | C6   | INH | V | 1   | 7.422   | 38.514 | 70.154 | 1.00 | 38.70  |
|    | ATOM | 4891 | C5   | INH | V | 1   | 7.571   | 39.820 | 69.689 | 1.00 | 37.05  |
|    | ATOM | 4892 | C4   | INH | V | 1   | 7.901   | 40.062 | 68.354 | 1.00 | 31.41  |
| 40 | ATOM | 4893 | C3   | INH | V | 1   | 8.091   | 38.967 | 67.505 | 1.00 | 35.48  |
|    | ATOM | 4894 | C2   | INH | V | 1   | 7.944   | 37.650 | 67.949 | 1.00 | 31.90  |
|    | ATOM | 4895 | C1   | INH | V | 1   | 7.611   | 37.434 | 69.286 | 1.00 | 36.93  |
|    | ATOM | 4896 | C7   | INH | V | 1   | 8.071   | 41.463 | 67.833 | 1.00 | 32.28  |
|    | ATOM | 4897 | O1   | INH | V | 1   | 8.288   | 41.443 | 66.485 | 1.00 | 37.06  |
|    | ATOM | 4898 | C8   | INH | V | 1   | 9.584   | 41.740 | 66.129 | 1.00 | 32.34  |
| 45 | ATOM | 4899 | C9   | INH | V | 1   | 9.825   | 42.911 | 65.416 | 1.00 | 31.03  |
|    | ATOM | 4900 | C10  | INH | V | 1   | 11.127  | 43.216 | 65.023 | 1.00 | 33.64  |
|    | ATOM | 4901 | C11  | INH | V | 1   | 12.194  | 42.381 | 65.339 | 1.00 | 31.88  |
|    | ATOM | 4902 | C12  | INH | V | 1   | 11.928  | 41.198 | 66.028 | 1.00 | 31.07  |
|    | ATOM | 4903 | C13  | INH | V | 1   | 10.630  | 40.858 | 66.412 | 1.00 | 28.70  |
| 50 | ATOM | 4904 | C14  | INH | V | 1   | 13.587  | 42.710 | 64.882 | 1.00 | 32.51  |
|    | ATOM | 4905 | C15  | INH | V | 1   | 14.260  | 41.560 | 64.121 | 1.00 | 34.69  |
|    | ATOM | 4906 | C16  | INH | V | 1   | 15.683  | 41.849 | 63.754 | 1.00 | 28.88  |
|    | ATOM | 4907 | S1   | INH | V | 1   | 16.605  | 40.755 | 64.790 | 1.00 | 29.16  |
|    | ATOM | 4908 | N1   | INH | V | 1   | 13.497  | 40.805 | 63.099 | 1.00 | 30.69  |
| 55 | ATOM | 4909 | O    | HOH | W | 1   | 44.463  | 49.888 | 77.523 | 1.00 | 46.91  |
|    | ATOM | 4910 | O    | HOH | W | 2   | 13.469  | 27.803 | 78.018 | 1.00 | 20.07  |
|    | ATOM | 4911 | O    | HOH | W | 3   | 4.225   | 69.721 | 58.393 | 1.00 | 27.76  |
|    | ATOM | 4912 | O    | HOH | W | 4   | 15.603  | 28.826 | 61.823 | 1.00 | 22.81  |
|    | ATOM | 4913 | O    | HOH | W | 5   | 22.862  | 26.624 | 42.874 | 1.00 | 53.05  |
| 60 | ATOM | 4914 | O    | HOH | W | 6   | 8.423   | 46.452 | 57.584 | 1.00 | 32.22  |
|    | ATOM | 4915 | O    | HOH | W | 7   | 17.904  | 46.550 | 68.524 | 1.00 | 31.91  |
|    | ATOM | 4916 | O    | HOH | W | 8   | 22.979  | 45.895 | 83.716 | 1.00 | 39.37  |
|    | ATOM | 4917 | O    | HOH | W | 9   | 17.707  | 39.158 | 55.643 | 1.00 | 25.27  |
|    | ATOM | 4918 | O    | HOH | W | 10  | 12.439  | 36.303 | 59.209 | 1.00 | 31.46  |



|    |      |      |   |     |   |    |         |        |         |      |       |
|----|------|------|---|-----|---|----|---------|--------|---------|------|-------|
|    | ATOM | 4919 | O | HOH | W | 11 | 17.367  | 62.730 | 50.320  | 1.00 | 37.74 |
|    | ATOM | 4920 | O | HOH | W | 12 | 42.823  | 52.642 | 90.552  | 1.00 | 53.80 |
|    | ATOM | 4921 | O | HOH | W | 13 | 34.337  | 45.508 | 97.419  | 1.00 | 57.99 |
| 5  | ATOM | 4922 | O | HOH | W | 14 | 6.726   | 27.119 | 48.459  | 1.00 | 62.29 |
|    | ATOM | 4923 | O | HOH | W | 15 | -0.093  | 30.159 | 71.746  | 1.00 | 29.96 |
|    | ATOM | 4924 | O | HOH | W | 16 | -19.673 | 44.016 | 58.682  | 1.00 | 58.64 |
|    | ATOM | 4925 | O | HOH | W | 17 | 16.563  | 26.790 | 80.837  | 1.00 | 38.62 |
|    | ATOM | 4926 | O | HOH | W | 18 | 10.281  | 35.677 | 88.518  | 1.00 | 26.01 |
| 10 | ATOM | 4927 | O | HOH | W | 19 | 20.973  | 35.691 | 44.774  | 1.00 | 49.50 |
|    | ATOM | 4928 | O | HOH | W | 20 | 0.996   | 19.571 | 53.713  | 1.00 | 67.39 |
|    | ATOM | 4929 | O | HOH | W | 21 | 20.424  | 37.014 | 85.845  | 1.00 | 39.54 |
|    | ATOM | 4930 | O | HOH | W | 22 | -2.498  | 35.905 | 53.781  | 1.00 | 51.70 |
|    | ATOM | 4931 | O | HOH | W | 23 | 39.807  | 49.718 | 92.595  | 1.00 | 37.39 |
| 15 | ATOM | 4932 | O | HOH | W | 24 | 16.431  | 58.267 | 93.127  | 1.00 | 47.45 |
|    | ATOM | 4933 | O | HOH | W | 25 | 6.935   | 45.104 | 66.012  | 1.00 | 18.12 |
|    | ATOM | 4934 | O | HOH | W | 26 | 40.479  | 54.713 | 100.253 | 1.00 | 28.72 |
|    | ATOM | 4935 | O | HOH | W | 27 | 22.369  | 40.324 | 67.919  | 1.00 | 46.36 |
|    | ATOM | 4936 | O | HOH | W | 28 | 37.289  | 49.457 | 68.016  | 1.00 | 61.37 |
| 20 | ATOM | 4937 | O | HOH | W | 29 | 2.611   | 35.015 | 55.709  | 1.00 | 24.45 |
|    | ATOM | 4938 | O | HOH | W | 30 | 41.088  | 62.590 | 98.644  | 1.00 | 65.38 |
|    | ATOM | 4939 | O | HOH | W | 31 | 17.369  | 55.024 | 87.465  | 1.00 | 24.22 |
|    | ATOM | 4940 | O | HOH | W | 32 | 25.433  | 20.198 | 55.692  | 1.00 | 44.61 |
|    | ATOM | 4941 | O | HOH | W | 33 | 3.890   | 42.770 | 66.651  | 1.00 | 22.34 |
| 25 | ATOM | 4942 | O | HOH | W | 34 | 3.934   | 63.391 | 62.592  | 1.00 | 60.69 |
|    | ATOM | 4943 | O | HOH | W | 35 | 22.280  | 41.610 | 86.289  | 1.00 | 74.20 |
|    | ATOM | 4944 | O | HOH | W | 36 | 22.631  | 46.401 | 90.078  | 1.00 | 47.44 |
|    | ATOM | 4945 | O | HOH | W | 37 | 33.442  | 20.227 | 64.569  | 1.00 | 55.41 |
|    | ATOM | 4946 | O | HOH | W | 38 | 39.834  | 28.974 | 75.602  | 1.00 | 41.72 |
| 30 | ATOM | 4947 | O | HOH | W | 39 | 35.232  | 47.140 | 54.186  | 1.00 | 37.08 |
|    | ATOM | 4948 | O | HOH | W | 40 | 36.003  | 57.784 | 57.893  | 1.00 | 43.05 |
|    | ATOM | 4949 | O | HOH | W | 41 | 37.216  | 27.438 | 74.564  | 1.00 | 50.79 |
|    | ATOM | 4950 | O | HOH | W | 42 | 17.770  | 67.012 | 77.183  | 1.00 | 45.78 |
|    | ATOM | 4951 | O | HOH | W | 43 | 5.341   | 31.286 | 78.127  | 1.00 | 25.34 |
| 35 | ATOM | 4952 | O | HOH | W | 44 | 33.535  | 32.503 | 52.063  | 1.00 | 56.13 |
|    | ATOM | 4953 | O | HOH | W | 45 | 25.477  | 33.146 | 44.610  | 1.00 | 65.43 |
|    | ATOM | 4954 | O | HOH | W | 46 | 16.235  | 37.438 | 52.628  | 1.00 | 32.10 |
|    | ATOM | 4955 | O | HOH | W | 47 | 28.791  | 14.101 | 63.316  | 1.00 | 46.67 |
|    | ATOM | 4956 | O | HOH | W | 48 | 10.230  | 24.992 | 86.967  | 1.00 | 38.63 |
| 40 | ATOM | 4957 | O | HOH | W | 49 | 30.821  | 38.856 | 79.630  | 1.00 | 40.44 |
|    | ATOM | 4958 | O | HOH | W | 50 | 12.621  | 37.226 | 62.944  | 1.00 | 26.70 |
|    | ATOM | 4959 | O | HOH | W | 51 | 27.987  | 30.609 | 66.612  | 1.00 | 33.55 |
|    | ATOM | 4960 | O | HOH | W | 52 | 34.459  | 28.696 | 64.242  | 1.00 | 51.01 |
|    | ATOM | 4961 | O | HOH | W | 53 | 34.969  | 62.270 | 91.179  | 1.00 | 68.20 |
| 45 | ATOM | 4962 | O | HOH | W | 54 | 33.631  | 30.717 | 62.396  | 1.00 | 41.64 |
|    | ATOM | 4963 | O | HOH | W | 55 | 43.987  | 48.530 | 91.269  | 1.00 | 50.99 |
|    | ATOM | 4964 | O | HOH | W | 56 | 23.412  | 28.584 | 85.186  | 1.00 | 69.23 |
|    | ATOM | 4965 | O | HOH | W | 57 | 39.834  | 28.057 | 72.257  | 1.00 | 81.00 |
|    | ATOM | 4966 | O | HOH | W | 58 | 2.892   | 25.685 | 69.907  | 1.00 | 38.96 |
| 50 | ATOM | 4967 | O | HOH | W | 59 | 10.284  | 47.120 | 72.671  | 1.00 | 40.28 |
|    | ATOM | 4968 | O | HOH | W | 60 | 32.645  | 39.037 | 76.746  | 1.00 | 21.71 |
|    | ATOM | 4969 | O | HOH | W | 61 | 43.535  | 48.019 | 95.228  | 1.00 | 37.69 |
|    | ATOM | 4970 | O | HOH | W | 62 | 11.991  | 51.053 | 43.479  | 1.00 | 41.05 |
|    | ATOM | 4971 | O | HOH | W | 63 | 18.329  | 56.527 | 89.388  | 1.00 | 28.51 |
| 55 | ATOM | 4972 | O | HOH | W | 64 | 16.555  | 9.309  | 68.875  | 1.00 | 89.05 |
|    | ATOM | 4973 | O | HOH | W | 65 | 23.741  | 44.759 | 73.150  | 1.00 | 38.43 |
|    | ATOM | 4974 | O | HOH | W | 66 | 19.093  | 53.805 | 41.239  | 1.00 | 55.25 |
|    | ATOM | 4975 | O | HOH | W | 67 | 31.750  | 60.369 | 56.933  | 1.00 | 92.26 |
|    | ATOM | 4976 | O | HOH | W | 68 | 24.836  | 68.428 | 80.926  | 1.00 | 59.25 |
| 60 | ATOM | 4977 | O | HOH | W | 69 | -21.014 | 19.446 | 48.342  | 1.00 | 52.24 |
|    | ATOM | 4978 | O | HOH | W | 70 | 11.318  | 68.028 | 86.566  | 1.00 | 77.81 |
|    | ATOM | 4979 | O | HOH | W | 71 | 5.312   | 60.076 | 63.511  | 1.00 | 36.83 |
|    | ATOM | 4980 | O | HOH | W | 72 | 7.689   | 20.219 | 84.680  | 1.00 | 32.24 |
|    | ATOM | 4981 | O | HOH | W | 73 | 34.988  | 44.708 | 64.746  | 1.00 | 40.73 |
|    | ATOM | 4982 | O | HOH | W | 74 | 10.614  | 49.644 | 41.337  | 1.00 | 38.90 |



|    |      |      |   |     |   |     |         |        |         |      |       |
|----|------|------|---|-----|---|-----|---------|--------|---------|------|-------|
|    | ATOM | 4983 | O | HOH | W | 75  | 19.349  | 42.973 | 64.739  | 1.00 | 54.53 |
|    | ATOM | 4984 | O | HOH | W | 76  | 35.916  | 30.862 | 80.753  | 1.00 | 55.38 |
|    | ATOM | 4985 | O | HOH | W | 77  | 9.666   | 26.046 | 46.603  | 1.00 | 40.09 |
| 5  | ATOM | 4986 | O | HOH | W | 78  | -10.171 | 46.751 | 60.237  | 1.00 | 29.78 |
|    | ATOM | 4987 | O | HOH | W | 79  | 46.751  | 58.883 | 86.875  | 1.00 | 35.92 |
|    | ATOM | 4988 | O | HOH | W | 80  | 19.320  | 32.528 | 51.000  | 1.00 | 33.36 |
|    | ATOM | 4989 | O | HOH | W | 81  | 28.815  | 39.568 | 66.176  | 1.00 | 59.19 |
|    | ATOM | 4990 | O | HOH | W | 82  | 38.207  | 35.773 | 73.585  | 1.00 | 17.81 |
| 10 | ATOM | 4991 | O | HOH | W | 83  | 23.802  | 33.925 | 75.175  | 1.00 | 25.19 |
|    | ATOM | 4992 | O | HOH | W | 84  | 42.241  | 51.290 | 99.896  | 1.00 | 15.88 |
|    | ATOM | 4993 | O | HOH | W | 85  | 3.751   | 36.678 | 58.842  | 1.00 | 24.97 |
|    | ATOM | 4994 | O | HOH | W | 86  | -7.009  | 40.341 | 62.580  | 1.00 | 25.39 |
|    | ATOM | 4995 | O | HOH | W | 87  | 11.735  | 58.910 | 68.155  | 1.00 | 39.70 |
| 15 | ATOM | 4996 | O | HOH | W | 88  | 13.986  | 52.835 | 42.224  | 1.00 | 50.91 |
|    | ATOM | 4997 | O | HOH | W | 89  | 1.452   | 46.541 | 69.459  | 1.00 | 35.03 |
|    | ATOM | 4998 | O | HOH | W | 90  | -1.938  | 55.310 | 56.971  | 1.00 | 28.10 |
|    | ATOM | 4999 | O | HOH | W | 91  | 13.801  | 66.947 | 52.600  | 1.00 | 38.65 |
|    | ATOM | 5000 | O | HOH | W | 92  | 21.594  | 47.218 | 79.203  | 1.00 | 30.31 |
| 20 | ATOM | 5001 | O | HOH | W | 93  | 10.639  | 58.632 | 90.827  | 1.00 | 43.78 |
|    | ATOM | 5002 | O | HOH | W | 94  | 33.335  | 53.550 | 68.086  | 1.00 | 37.04 |
|    | ATOM | 5003 | O | HOH | W | 95  | -1.984  | 28.738 | 60.212  | 1.00 | 31.56 |
|    | ATOM | 5004 | O | HOH | W | 96  | -4.958  | 51.055 | 59.250  | 1.00 | 34.00 |
|    | ATOM | 5005 | O | HOH | W | 97  | 17.610  | 39.701 | 51.503  | 1.00 | 28.27 |
| 25 | ATOM | 5006 | O | HOH | W | 98  | 10.686  | 54.166 | 67.565  | 1.00 | 37.68 |
|    | ATOM | 5007 | O | HOH | W | 99  | 20.567  | 43.859 | 78.621  | 1.00 | 41.57 |
|    | ATOM | 5008 | O | HOH | W | 100 | 7.013   | 22.332 | 69.109  | 1.00 | 28.72 |
|    | ATOM | 5009 | O | HOH | W | 101 | 10.097  | 53.225 | 78.477  | 1.00 | 35.68 |
|    | ATOM | 5010 | O | HOH | W | 102 | 10.849  | 31.404 | 53.014  | 1.00 | 32.22 |
| 30 | ATOM | 5011 | O | HOH | W | 103 | 42.381  | 59.035 | 94.728  | 1.00 | 36.00 |
|    | ATOM | 5012 | O | HOH | W | 104 | 17.234  | 41.111 | 54.082  | 1.00 | 33.65 |
|    | ATOM | 5013 | O | HOH | W | 105 | 26.902  | 62.025 | 81.989  | 1.00 | 34.70 |
|    | ATOM | 5014 | O | HOH | W | 106 | -14.313 | 49.559 | 56.204  | 1.00 | 54.36 |
|    | ATOM | 5015 | O | HOH | W | 107 | 41.646  | 57.501 | 101.015 | 1.00 | 68.12 |
| 35 | ATOM | 5016 | O | HOH | W | 108 | 26.759  | 43.000 | 47.219  | 1.00 | 32.69 |
|    | ATOM | 5017 | O | HOH | W | 109 | 16.624  | 48.119 | 46.545  | 1.00 | 38.64 |
|    | ATOM | 5018 | O | HOH | W | 110 | 26.159  | 32.793 | 75.230  | 1.00 | 24.77 |
|    | ATOM | 5019 | O | HOH | W | 111 | 2.101   | 33.468 | 67.006  | 1.00 | 31.50 |
|    | ATOM | 5020 | O | HOH | W | 112 | 38.114  | 36.374 | 87.451  | 1.00 | 44.06 |
| 40 | ATOM | 5021 | O | HOH | W | 113 | 13.211  | 29.810 | 61.356  | 1.00 | 33.81 |
|    | ATOM | 5022 | O | HOH | W | 114 | -3.064  | 37.863 | 40.673  | 1.00 | 37.92 |
|    | ATOM | 5023 | O | HOH | W | 115 | 15.007  | 47.948 | 69.488  | 1.00 | 28.23 |
|    | ATOM | 5024 | O | HOH | W | 116 | 27.101  | 66.633 | 80.518  | 1.00 | 41.24 |
|    | ATOM | 5025 | O | HOH | W | 117 | 11.870  | 38.304 | 43.174  | 1.00 | 40.85 |
| 45 | ATOM | 5026 | O | HOH | W | 118 | -13.844 | 25.597 | 58.258  | 1.00 | 53.75 |
|    | ATOM | 5027 | O | HOH | W | 119 | 2.929   | 41.135 | 59.858  | 1.00 | 36.49 |
|    | ATOM | 5028 | O | HOH | W | 120 | 24.890  | 45.490 | 82.167  | 1.00 | 41.65 |
|    | ATOM | 5029 | O | HOH | W | 121 | 36.062  | 59.335 | 75.090  | 1.00 | 38.82 |
|    | ATOM | 5030 | O | HOH | W | 122 | -10.715 | 32.037 | 61.699  | 1.00 | 78.82 |
| 50 | ATOM | 5031 | O | HOH | W | 123 | -2.646  | 25.492 | 60.812  | 1.00 | 48.40 |
|    | ATOM | 5032 | O | HOH | W | 124 | -8.948  | 46.831 | 63.556  | 1.00 | 48.06 |
|    | ATOM | 5033 | O | HOH | W | 125 | -17.843 | 39.367 | 36.020  | 1.00 | 35.80 |
|    | ATOM | 5034 | O | HOH | W | 126 | 2.218   | 57.766 | 62.253  | 1.00 | 44.61 |
|    | ATOM | 5035 | O | HOH | W | 127 | 10.736  | 62.766 | 64.366  | 1.00 | 55.84 |
| 55 | ATOM | 5036 | O | HOH | W | 128 | 0.884   | 35.562 | 63.963  | 1.00 | 44.14 |
|    | ATOM | 5037 | O | HOH | W | 129 | 19.165  | 59.557 | 60.644  | 1.00 | 47.82 |
|    | ATOM | 5038 | O | HOH | W | 130 | 1.546   | 27.875 | 68.443  | 1.00 | 39.69 |
|    | ATOM | 5039 | O | HOH | W | 131 | 5.497   | 26.285 | 76.668  | 1.00 | 44.47 |
|    | ATOM | 5040 | O | HOH | W | 132 | 14.505  | 36.538 | 88.996  | 1.00 | 40.00 |
| 60 | ATOM | 5041 | O | HOH | W | 133 | 8.534   | 28.713 | 88.519  | 1.00 | 46.55 |
|    | ATOM | 5042 | O | HOH | W | 134 | 6.125   | 45.267 | 77.959  | 1.00 | 45.57 |
|    | ATOM | 5043 | O | HOH | W | 135 | 26.016  | 18.543 | 78.878  | 1.00 | 51.65 |
|    | ATOM | 5044 | O | HOH | W | 136 | 33.880  | 23.025 | 70.739  | 1.00 | 46.95 |
|    | ATOM | 5045 | O | HOH | W | 137 | 19.230  | 26.073 | 49.998  | 1.00 | 51.97 |
|    | ATOM | 5046 | O | HOH | W | 138 | 41.563  | 41.085 | 77.326  | 1.00 | 43.14 |



|    |      |      |   |           |         |        |        |      |       |
|----|------|------|---|-----------|---------|--------|--------|------|-------|
|    | ATOM | 5047 | O | HOH W 139 | 39.187  | 63.067 | 75.380 | 1.00 | 56.52 |
|    | ATOM | 5048 | O | HOH W 140 | 26.878  | 54.491 | 67.203 | 1.00 | 42.14 |
|    | ATOM | 5049 | O | HOH W 141 | 22.988  | 62.189 | 74.174 | 1.00 | 48.31 |
| 5  | ATOM | 5050 | O | HOH W 142 | 25.190  | 62.803 | 71.067 | 1.00 | 67.16 |
|    | ATOM | 5051 | O | HOH W 143 | 18.598  | 45.126 | 81.949 | 1.00 | 53.80 |
|    | ATOM | 5052 | O | HOH W 144 | 19.782  | 53.129 | 90.556 | 1.00 | 48.73 |
|    | ATOM | 5053 | O | HOH W 145 | 21.735  | 48.367 | 86.454 | 1.00 | 40.39 |
|    | ATOM | 5054 | O | HOH W 146 | 25.707  | 57.012 | 93.476 | 1.00 | 53.61 |
| 10 | ATOM | 5055 | O | HOH W 147 | 22.832  | 62.085 | 93.149 | 1.00 | 46.02 |
|    | ATOM | 5056 | O | HOH W 148 | 25.725  | 67.203 | 89.990 | 1.00 | 75.23 |
|    | ATOM | 5057 | O | HOH W 149 | 10.773  | 53.653 | 85.697 | 1.00 | 50.65 |
|    | ATOM | 5058 | O | HOH W 150 | 4.221   | 58.449 | 86.608 | 1.00 | 49.23 |
|    | ATOM | 5059 | O | HOH W 151 | 7.790   | 72.096 | 84.410 | 1.00 | 51.10 |
| 15 | ATOM | 5060 | O | HOH W 152 | 2.387   | 58.282 | 67.835 | 1.00 | 33.29 |
|    | ATOM | 5061 | O | HOH W 153 | 0.921   | 49.551 | 69.095 | 1.00 | 59.60 |
|    | ATOM | 5062 | O | HOH W 154 | 8.722   | 45.171 | 71.561 | 1.00 | 46.56 |
|    | ATOM | 5063 | O | HOH W 155 | 6.422   | 47.947 | 81.081 | 1.00 | 57.56 |
|    | ATOM | 5064 | O | HOH W 156 | 15.936  | 56.908 | 55.129 | 1.00 | 43.33 |
| 20 | ATOM | 5065 | O | HOH W 157 | 3.032   | 19.635 | 62.453 | 1.00 | 80.38 |
|    | ATOM | 5066 | O | HOH W 158 | -4.228  | 58.058 | 47.057 | 1.00 | 39.66 |
|    | ATOM | 5067 | O | HOH W 159 | 1.197   | 41.002 | 78.942 | 1.00 | 57.22 |
|    | ATOM | 5068 | O | HOH W 160 | 1.259   | 43.651 | 68.100 | 1.00 | 37.94 |
|    | ATOM | 5069 | O | HOH W 161 | 25.799  | 64.833 | 56.690 | 1.00 | 38.96 |
| 25 | ATOM | 5070 | O | HOH W 162 | -11.853 | 45.054 | 45.070 | 1.00 | 38.38 |
|    | ATOM | 5071 | O | HOH W 163 | 40.159  | 31.033 | 78.548 | 1.00 | 75.36 |
|    | ATOM | 5072 | O | HOH W 164 | 21.477  | 20.377 | 79.349 | 1.00 | 35.96 |
|    | ATOM | 5073 | O | HOH W 165 | 26.347  | 44.558 | 72.803 | 1.00 | 42.21 |
|    | ATOM | 5074 | O | HOH W 166 | 16.446  | 61.207 | 59.687 | 1.00 | 39.70 |
| 30 | ATOM | 5075 | O | HOH W 167 | 27.695  | 64.216 | 82.410 | 1.00 | 44.71 |
|    | ATOM | 5076 | O | HOH W 168 | -2.998  | 57.511 | 34.738 | 1.00 | 45.35 |
|    | ATOM | 5077 | O | HOH W 169 | 6.608   | 51.527 | 60.826 | 1.00 | 39.48 |
|    | ATOM | 5078 | O | HOH W 170 | 31.104  | 28.934 | 81.337 | 1.00 | 43.19 |
|    | ATOM | 5079 | O | HOH W 171 | 10.135  | 28.233 | 45.533 | 1.00 | 41.24 |
| 35 | ATOM | 5080 | O | HOH W 172 | 8.201   | 43.960 | 75.322 | 1.00 | 37.71 |
|    | ATOM | 5081 | O | HOH W 173 | 13.799  | 66.601 | 85.597 | 1.00 | 34.74 |
|    | ATOM | 5082 | O | HOH W 174 | 16.664  | 53.670 | 65.006 | 1.00 | 43.69 |
|    | ATOM | 5083 | O | HOH W 175 | 18.301  | 47.296 | 43.793 | 1.00 | 45.84 |
|    | ATOM | 5084 | O | HOH W 176 | 11.717  | 61.868 | 52.648 | 1.00 | 34.93 |
| 40 | ATOM | 5085 | O | HOH W 177 | 29.516  | 23.822 | 76.838 | 1.00 | 51.50 |
|    | ATOM | 5086 | O | HOH W 178 | 39.940  | 60.509 | 78.535 | 1.00 | 46.33 |
|    | ATOM | 5087 | O | HOH W 179 | -1.803  | 44.974 | 37.278 | 1.00 | 52.56 |
|    | ATOM | 5088 | O | HOH W 180 | 7.343   | 47.305 | 65.468 | 1.00 | 47.27 |
|    | ATOM | 5089 | O | HOH W 181 | 17.912  | 15.338 | 81.793 | 1.00 | 50.08 |
| 45 | ATOM | 5090 | O | HOH W 182 | -4.631  | 55.917 | 82.183 | 1.00 | 65.36 |
|    | ATOM | 5091 | O | HOH W 183 | 32.973  | 42.656 | 86.667 | 1.00 | 43.97 |
|    | ATOM | 5092 | O | HOH W 184 | -1.834  | 36.784 | 71.040 | 1.00 | 45.10 |
|    | ATOM | 5093 | O | HOH W 185 | -4.519  | 34.633 | 71.838 | 1.00 | 43.99 |
|    | ATOM | 5094 | O | HOH W 186 | 4.518   | 68.554 | 71.661 | 1.00 | 46.99 |
| 50 | ATOM | 5095 | O | HOH W 187 | 2.774   | 37.503 | 61.490 | 1.00 | 45.81 |
|    | ATOM | 5096 | O | HOH W 188 | 31.770  | 43.526 | 51.410 | 1.00 | 58.02 |
|    | ATOM | 5097 | O | HOH W 189 | 5.471   | 43.861 | 38.891 | 1.00 | 49.43 |
|    | ATOM | 5098 | O | HOH W 190 | 11.934  | 58.219 | 70.811 | 1.00 | 49.96 |
|    | ATOM | 5099 | O | HOH W 191 | 33.112  | 26.203 | 70.484 | 1.00 | 60.03 |
| 55 | ATOM | 5100 | O | HOH W 192 | 30.914  | 43.017 | 70.613 | 1.00 | 73.23 |
|    | ATOM | 5101 | O | HOH W 193 | 0.400   | 39.300 | 39.714 | 1.00 | 65.37 |
|    | ATOM | 5102 | O | HOH W 194 | 48.247  | 56.159 | 86.370 | 1.00 | 60.09 |
|    | ATOM | 5103 | O | HOH W 195 | 12.359  | 59.992 | 62.698 | 1.00 | 53.57 |
|    | ATOM | 5104 | O | HOH W 196 | 11.149  | 17.504 | 78.264 | 1.00 | 54.43 |
| 60 | ATOM | 5105 | O | HOH W 197 | -4.284  | 31.953 | 60.991 | 1.00 | 47.12 |
|    | ATOM | 5106 | O | HOH W 198 | 29.888  | 35.624 | 82.772 | 1.00 | 52.16 |
|    | ATOM | 5107 | O | HOH W 199 | 14.388  | 39.115 | 89.656 | 1.00 | 47.93 |
|    | ATOM | 5108 | O | HOH W 200 | -8.529  | 51.475 | 47.745 | 1.00 | 61.00 |
|    | ATOM | 5109 | O | HOH W 201 | -15.572 | 53.338 | 52.008 | 1.00 | 72.42 |
|    | ATOM | 5110 | O | HOH W 202 | 24.319  | 38.590 | 87.128 | 1.00 | 50.03 |







Table 11: Structure coordinates of LTA<sub>4</sub> hydrolase-hydroxamic acid complex

| CRYST | 67.770 | 132.470 | 83.700 | 90.00 | 90.00 | 90.00  | P21212 |                    |
|-------|--------|---------|--------|-------|-------|--------|--------|--------------------|
|       | Atom   | res.    | Chain  | No.   | x     | y      | z      | occ B-factor       |
| 5     | ATOM   | 1       | N      | PRO A | 1     | -2.215 | 16.942 | 65.912 1.00 98.67  |
|       | ATOM   | 2       | CA     | PRO A | 1     | -2.492 | 18.109 | 66.739 1.00 96.57  |
|       | ATOM   | 3       | C      | PRO A | 1     | -1.985 | 19.345 | 66.046 1.00 90.92  |
|       | ATOM   | 4       | O      | PRO A | 1     | -0.791 | 19.459 | 65.732 1.00 87.94  |
|       | ATOM   | 5       | CB     | PRO A | 1     | -1.747 | 17.907 | 68.073 1.00 98.18  |
| 10    | ATOM   | 6       | CG     | PRO A | 1     | -1.000 | 16.573 | 67.973 1.00 100.00 |
|       | ATOM   | 7       | CD     | PRO A | 1     | -1.249 | 16.011 | 66.573 1.00 97.96  |
|       | ATOM   | 8       | N      | GLU A | 2     | -2.895 | 20.262 | 65.790 1.00 83.08  |
|       | ATOM   | 9       | CA     | GLU A | 2     | -2.492 | 21.448 | 65.116 1.00 81.25  |
|       | ATOM   | 10      | C      | GLU A | 2     | -1.948 | 22.471 | 66.074 1.00 80.21  |
| 15    | ATOM   | 11      | O      | GLU A | 2     | -2.444 | 22.625 | 67.189 1.00 80.90  |
|       | ATOM   | 12      | CB     | GLU A | 2     | -3.549 | 22.038 | 64.168 1.00 82.10  |
|       | ATOM   | 13      | CG     | GLU A | 2     | -2.895 | 22.838 | 63.023 1.00 92.94  |
|       | ATOM   | 14      | CD     | GLU A | 2     | -1.451 | 22.466 | 62.778 1.00 95.77  |
| 20    | ATOM   | 15      | OE1    | GLU A | 2     | -0.520 | 23.237 | 62.917 1.00 94.64  |
|       | ATOM   | 16      | OE2    | GLU A | 2     | -1.307 | 21.231 | 62.383 1.00 74.00  |
|       | ATOM   | 17      | N      | ILE A | 3     | -0.898 | 23.141 | 65.624 1.00 69.91  |
|       | ATOM   | 18      | CA     | ILE A | 3     | -0.300 | 24.192 | 66.393 1.00 66.19  |
|       | ATOM   | 19      | C      | ILE A | 3     | -1.124 | 25.431 | 66.042 1.00 60.35  |
|       | ATOM   | 20      | O      | ILE A | 3     | -1.438 | 25.713 | 64.866 1.00 60.57  |
| 25    | ATOM   | 21      | CB     | ILE A | 3     | 1.215  | 24.316 | 66.167 1.00 69.46  |
|       | ATOM   | 22      | CG1    | ILE A | 3     | 1.919  | 23.117 | 66.809 1.00 69.22  |
|       | ATOM   | 23      | CG2    | ILE A | 3     | 1.772  | 25.604 | 66.769 1.00 70.57  |
|       | ATOM   | 24      | CD1    | ILE A | 3     | 2.674  | 23.468 | 68.090 1.00 67.16  |
| 30    | ATOM   | 25      | N      | VAL A | 4     | -1.546 | 26.135 | 67.071 1.00 47.12  |
|       | ATOM   | 26      | CA     | VAL A | 4     | -2.372 | 27.296 | 66.856 1.00 43.66  |
|       | ATOM   | 27      | C      | VAL A | 4     | -1.621 | 28.601 | 66.943 1.00 36.61  |
|       | ATOM   | 28      | O      | VAL A | 4     | -0.804 | 28.799 | 67.843 1.00 33.97  |
|       | ATOM   | 29      | CB     | VAL A | 4     | -3.580 | 27.282 | 67.811 1.00 46.37  |
| 35    | ATOM   | 30      | CG1    | VAL A | 4     | -4.296 | 28.636 | 67.855 1.00 44.31  |
|       | ATOM   | 31      | CG2    | VAL A | 4     | -4.552 | 26.203 | 67.353 1.00 45.89  |
|       | ATOM   | 32      | N      | ASP A | 5     | -1.920 | 29.496 | 65.997 1.00 25.42  |
|       | ATOM   | 33      | CA     | ASP A | 5     | -1.311 | 30.793 | 66.050 1.00 22.70  |
|       | ATOM   | 34      | C      | ASP A | 5     | -2.262 | 31.630 | 66.874 1.00 26.31  |
| 40    | ATOM   | 35      | O      | ASP A | 5     | -3.285 | 32.069 | 66.397 1.00 25.00  |
|       | ATOM   | 36      | CB     | ASP A | 5     | -1.083 | 31.454 | 64.687 1.00 23.91  |
|       | ATOM   | 37      | CG     | ASP A | 5     | -0.248 | 32.685 | 64.868 1.00 28.48  |
|       | ATOM   | 38      | OD1    | ASP A | 5     | -0.199 | 33.272 | 65.935 1.00 27.12  |
|       | ATOM   | 39      | OD2    | ASP A | 5     | 0.383  | 33.068 | 63.776 1.00 23.01  |
| 45    | ATOM   | 40      | N      | THR A | 6     | -1.942 | 31.792 | 68.144 1.00 25.96  |
|       | ATOM   | 41      | CA     | THR A | 6     | -2.799 | 32.525 | 69.029 1.00 23.74  |
|       | ATOM   | 42      | C      | THR A | 6     | -2.689 | 34.005 | 68.859 1.00 27.92  |
|       | ATOM   | 43      | O      | THR A | 6     | -3.169 | 34.763 | 69.701 1.00 31.80  |
|       | ATOM   | 44      | CB     | THR A | 6     | -2.629 | 32.111 | 70.483 1.00 25.94  |
| 50    | ATOM   | 45      | OG1    | THR A | 6     | -1.315 | 32.422 | 70.891 1.00 40.88  |
|       | ATOM   | 46      | CG2    | THR A | 6     | -2.867 | 30.609 | 70.627 1.00 29.05  |
|       | ATOM   | 47      | N      | CYS A | 7     | -2.068 | 34.442 | 67.779 1.00 23.72  |
|       | ATOM   | 48      | CA     | CYS A | 7     | -1.967 | 35.893 | 67.566 1.00 24.38  |
|       | ATOM   | 49      | C      | CYS A | 7     | -2.737 | 36.321 | 66.325 1.00 28.42  |
| 55    | ATOM   | 50      | O      | CYS A | 7     | -2.766 | 37.475 | 65.965 1.00 27.59  |
|       | ATOM   | 51      | CB     | CYS A | 7     | -0.516 | 36.435 | 67.449 1.00 23.86  |
|       | ATOM   | 52      | SG     | CYS A | 7     | 0.510  | 36.080 | 68.886 1.00 29.33  |
|       | ATOM   | 53      | N      | SER A | 8     | -3.324 | 35.370 | 65.638 1.00 27.23  |
|       | ATOM   | 54      | CA     | SER A | 8     | -4.020 | 35.686 | 64.419 1.00 25.64  |
| 60    | ATOM   | 55      | C      | SER A | 8     | -5.479 | 35.340 | 64.538 1.00 25.31  |
|       | ATOM   | 56      | O      | SER A | 8     | -5.867 | 34.421 | 65.273 1.00 22.83  |
|       | ATOM   | 57      | CB     | SER A | 8     | -3.368 | 34.908 | 63.278 1.00 26.35  |
|       | ATOM   | 58      | OG     | SER A | 8     | -4.090 | 35.105 | 62.093 1.00 29.02  |



|    |      |     |     |     |   |    |         |        |        |      |       |
|----|------|-----|-----|-----|---|----|---------|--------|--------|------|-------|
|    | ATOM | 59  | N   | LEU | A | 9  | -6.298  | 36.071 | 63.799 | 1.00 | 20.95 |
|    | ATOM | 60  | CA  | LEU | A | 9  | -7.720  | 35.750 | 63.869 | 1.00 | 20.81 |
|    | ATOM | 61  | C   | LEU | A | 9  | -8.188  | 35.158 | 62.554 | 1.00 | 24.77 |
| 5  | ATOM | 62  | O   | LEU | A | 9  | -9.364  | 34.872 | 62.381 | 1.00 | 28.22 |
|    | ATOM | 63  | CB  | LEU | A | 9  | -8.573  | 36.991 | 64.170 | 1.00 | 20.29 |
|    | ATOM | 64  | CG  | LEU | A | 9  | -8.171  | 37.744 | 65.434 | 1.00 | 21.06 |
|    | ATOM | 65  | CD1 | LEU | A | 9  | -8.875  | 39.088 | 65.438 | 1.00 | 22.40 |
|    | ATOM | 66  | CD2 | LEU | A | 9  | -8.576  | 36.926 | 66.656 | 1.00 | 15.77 |
| 10 | ATOM | 67  | N   | ALA | A | 10 | -7.240  | 35.040 | 61.630 | 1.00 | 22.60 |
|    | ATOM | 68  | CA  | ALA | A | 10 | -7.461  | 34.528 | 60.294 | 1.00 | 17.85 |
|    | ATOM | 69  | C   | ALA | A | 10 | -7.633  | 33.039 | 60.254 | 1.00 | 23.94 |
|    | ATOM | 70  | O   | ALA | A | 10 | -7.281  | 32.298 | 61.178 | 1.00 | 22.85 |
|    | ATOM | 71  | CB  | ALA | A | 10 | -6.291  | 34.891 | 59.397 | 1.00 | 15.48 |
| 15 | ATOM | 72  | N   | SER | A | 11 | -8.170  | 32.590 | 59.129 | 1.00 | 25.50 |
|    | ATOM | 73  | CA  | SER | A | 11 | -8.306  | 31.156 | 58.921 | 1.00 | 27.59 |
|    | ATOM | 74  | C   | SER | A | 11 | -6.887  | 30.575 | 58.992 | 1.00 | 25.13 |
|    | ATOM | 75  | O   | SER | A | 11 | -5.938  | 31.112 | 58.437 | 1.00 | 26.43 |
|    | ATOM | 76  | CB  | SER | A | 11 | -8.917  | 30.833 | 57.544 | 1.00 | 29.01 |
| 20 | ATOM | 77  | OG  | SER | A | 11 | -10.241 | 31.338 | 57.445 | 1.00 | 28.50 |
|    | ATOM | 78  | N   | PRO | A | 12 | -6.740  | 29.460 | 59.662 | 1.00 | 23.36 |
|    | ATOM | 79  | CA  | PRO | A | 12 | -5.445  | 28.827 | 59.798 | 1.00 | 20.96 |
|    | ATOM | 80  | C   | PRO | A | 12 | -4.949  | 28.121 | 58.533 | 1.00 | 34.02 |
|    | ATOM | 81  | O   | PRO | A | 12 | -5.743  | 27.764 | 57.646 | 1.00 | 34.95 |
| 25 | ATOM | 82  | CB  | PRO | A | 12 | -5.590  | 27.834 | 60.952 | 1.00 | 22.26 |
|    | ATOM | 83  | CG  | PRO | A | 12 | -7.080  | 27.652 | 61.201 | 1.00 | 29.49 |
|    | ATOM | 84  | CD  | PRO | A | 12 | -7.769  | 28.845 | 60.542 | 1.00 | 25.95 |
|    | ATOM | 85  | N   | ALA | A | 13 | -3.615  | 27.927 | 58.479 | 1.00 | 29.46 |
|    | ATOM | 86  | CA  | ALA | A | 13 | -2.922  | 27.276 | 57.385 | 1.00 | 25.81 |
|    | ATOM | 87  | C   | ALA | A | 13 | -3.531  | 25.912 | 57.109 | 1.00 | 27.87 |
| 30 | ATOM | 88  | O   | ALA | A | 13 | -3.320  | 25.321 | 56.072 | 1.00 | 30.10 |
|    | ATOM | 89  | CB  | ALA | A | 13 | -1.458  | 27.115 | 57.746 | 1.00 | 25.60 |
|    | ATOM | 90  | N   | SER | A | 14 | -4.288  | 25.389 | 58.038 | 1.00 | 20.61 |
|    | ATOM | 91  | CA  | SER | A | 14 | -4.876  | 24.090 | 57.814 | 1.00 | 24.37 |
| 35 | ATOM | 92  | C   | SER | A | 14 | -6.230  | 24.183 | 57.108 | 1.00 | 32.80 |
|    | ATOM | 93  | O   | SER | A | 14 | -6.831  | 23.183 | 56.733 | 1.00 | 35.15 |
|    | ATOM | 94  | CB  | SER | A | 14 | -5.031  | 23.366 | 59.137 | 1.00 | 29.06 |
|    | ATOM | 95  | OG  | SER | A | 14 | -5.775  | 24.180 | 60.037 | 1.00 | 31.14 |
|    | ATOM | 96  | N   | VAL | A | 15 | -6.721  | 25.392 | 56.944 | 1.00 | 24.99 |
| 40 | ATOM | 97  | CA  | VAL | A | 15 | -7.984  | 25.582 | 56.278 | 1.00 | 25.26 |
|    | ATOM | 98  | C   | VAL | A | 15 | -7.774  | 26.148 | 54.865 | 1.00 | 27.71 |
|    | ATOM | 99  | O   | VAL | A | 15 | -8.348  | 25.688 | 53.886 | 1.00 | 27.54 |
|    | ATOM | 100 | CB  | VAL | A | 15 | -8.876  | 26.466 | 57.127 | 1.00 | 29.72 |
|    | ATOM | 101 | CG1 | VAL | A | 15 | -9.999  | 27.045 | 56.271 | 1.00 | 30.81 |
| 45 | ATOM | 102 | CG2 | VAL | A | 15 | -9.411  | 25.656 | 58.298 | 1.00 | 27.89 |
|    | ATOM | 103 | N   | CYS | A | 16 | -6.921  | 27.144 | 54.764 | 1.00 | 20.14 |
|    | ATOM | 104 | CA  | CYS | A | 16 | -6.594  | 27.769 | 53.503 | 1.00 | 24.17 |
|    | ATOM | 105 | C   | CYS | A | 16 | -5.265  | 28.490 | 53.629 | 1.00 | 26.96 |
|    | ATOM | 106 | O   | CYS | A | 16 | -4.834  | 28.793 | 54.744 | 1.00 | 28.25 |
| 50 | ATOM | 107 | CB  | CYS | A | 16 | -7.703  | 28.694 | 52.944 | 1.00 | 28.08 |
|    | ATOM | 108 | SG  | CYS | A | 16 | -7.881  | 30.231 | 53.880 | 1.00 | 34.58 |
|    | ATOM | 109 | N   | ARG | A | 17 | -4.622  | 28.749 | 52.496 | 1.00 | 20.39 |
|    | ATOM | 110 | CA  | ARG | A | 17 | -3.344  | 29.409 | 52.520 | 1.00 | 22.15 |
|    | ATOM | 111 | C   | ARG | A | 17 | -3.186  | 30.347 | 51.365 | 1.00 | 26.96 |
| 55 | ATOM | 112 | O   | ARG | A | 17 | -3.415  | 30.002 | 50.202 | 1.00 | 23.44 |
|    | ATOM | 113 | CB  | ARG | A | 17 | -2.147  | 28.451 | 52.443 | 1.00 | 26.39 |
|    | ATOM | 114 | CG  | ARG | A | 17 | -2.231  | 27.181 | 53.264 | 1.00 | 24.30 |
|    | ATOM | 115 | CD  | ARG | A | 17 | -1.416  | 26.086 | 52.599 | 1.00 | 28.56 |
|    | ATOM | 116 | NE  | ARG | A | 17 | -0.772  | 25.134 | 53.510 | 1.00 | 51.45 |
| 60 | ATOM | 117 | CZ  | ARG | A | 17 | -1.392  | 24.225 | 54.263 | 1.00 | 69.75 |
|    | ATOM | 118 | NH1 | ARG | A | 17 | -2.693  | 24.086 | 54.287 | 1.00 | 72.82 |
|    | ATOM | 119 | NH2 | ARG | A | 17 | -0.694  | 23.418 | 55.032 | 1.00 | 48.88 |
|    | ATOM | 120 | N   | THR | A | 18 | -2.723  | 31.532 | 51.700 | 1.00 | 21.89 |
|    | ATOM | 121 | CA  | THR | A | 18 | -2.478  | 32.539 | 50.713 | 1.00 | 20.46 |
|    | ATOM | 122 | C   | THR | A | 18 | -1.200  | 32.197 | 50.007 | 1.00 | 27.00 |



|    |      |     |     |     |   |    |        |        |        |      |        |
|----|------|-----|-----|-----|---|----|--------|--------|--------|------|--------|
|    | ATOM | 123 | O   | THR | A | 18 | -0.207 | 31.923 | 50.662 | 1.00 | 26.28  |
|    | ATOM | 124 | CB  | THR | A | 18 | -2.370 | 33.949 | 51.337 | 1.00 | 21.64  |
|    | ATOM | 125 | OG1 | THR | A | 18 | -3.539 | 34.262 | 52.076 | 1.00 | 25.03  |
| 5  | ATOM | 126 | CG2 | THR | A | 18 | -2.164 | 34.944 | 50.211 | 1.00 | 21.73  |
|    | ATOM | 127 | N   | LYS | A | 19 | -1.235 | 32.203 | 48.677 | 1.00 | 22.54  |
|    | ATOM | 128 | CA  | LYS | A | 19 | -0.091 | 31.871 | 47.864 | 1.00 | 21.16  |
|    | ATOM | 129 | C   | LYS | A | 19 | 0.538  | 33.063 | 47.238 | 1.00 | 23.51  |
|    | ATOM | 130 | O   | LYS | A | 19 | 1.732  | 33.098 | 46.968 | 1.00 | 23.00  |
| 10 | ATOM | 131 | CB  | LYS | A | 19 | -0.557 | 30.976 | 46.740 | 1.00 | 24.60  |
|    | ATOM | 132 | CG  | LYS | A | 19 | -1.311 | 29.775 | 47.257 | 1.00 | 34.24  |
|    | ATOM | 133 | CD  | LYS | A | 19 | -0.944 | 29.419 | 48.688 | 1.00 | 65.32  |
|    | ATOM | 134 | CE  | LYS | A | 19 | 0.230  | 28.442 | 48.793 | 1.00 | 75.40  |
|    | ATOM | 135 | NZ  | LYS | A | 19 | 1.183  | 28.796 | 49.864 | 1.00 | 66.99  |
| 15 | ATOM | 136 | N   | HIS | A | 20 | -0.280 | 34.053 | 46.967 | 1.00 | 22.30  |
|    | ATOM | 137 | CA  | HIS | A | 20 | 0.201  | 35.250 | 46.309 | 1.00 | 20.94  |
|    | ATOM | 138 | C   | HIS | A | 20 | -0.588 | 36.484 | 46.673 | 1.00 | 23.90  |
|    | ATOM | 139 | O   | HIS | A | 20 | -1.779 | 36.414 | 47.022 | 1.00 | 23.31  |
|    | ATOM | 140 | CB  | HIS | A | 20 | 0.054  | 35.095 | 44.801 | 1.00 | 19.15  |
| 20 | ATOM | 141 | CG  | HIS | A | 20 | 0.888  | 36.085 | 44.129 | 1.00 | 20.96  |
|    | ATOM | 142 | ND1 | HIS | A | 20 | 2.258  | 36.003 | 44.163 | 1.00 | 22.60  |
|    | ATOM | 143 | CD2 | HIS | A | 20 | 0.538  | 37.198 | 43.437 | 1.00 | 24.10  |
|    | ATOM | 144 | CE1 | HIS | A | 20 | 2.725  | 37.040 | 43.496 | 1.00 | 23.71  |
|    | ATOM | 145 | NE2 | HIS | A | 20 | 1.708  | 37.784 | 43.025 | 1.00 | 24.51  |
| 25 | ATOM | 146 | N   | LEU | A | 21 | 0.105  | 37.600 | 46.594 | 1.00 | 26.18  |
|    | ATOM | 147 | CA  | LEU | A | 21 | -0.484 | 38.893 | 46.871 | 1.00 | 27.24  |
|    | ATOM | 148 | C   | LEU | A | 21 | -0.104 | 39.856 | 45.805 | 1.00 | 27.01  |
|    | ATOM | 149 | O   | LEU | A | 21 | 1.076  | 40.014 | 45.522 | 1.00 | 27.97  |
|    | ATOM | 150 | CB  | LEU | A | 21 | -0.064 | 39.501 | 48.215 | 1.00 | 28.80  |
| 30 | ATOM | 151 | CG  | LEU | A | 21 | -0.335 | 41.006 | 48.296 | 1.00 | 34.13  |
|    | ATOM | 152 | CD1 | LEU | A | 21 | -1.834 | 41.309 | 48.440 | 1.00 | 36.26  |
|    | ATOM | 153 | CD2 | LEU | A | 21 | 0.393  | 41.578 | 49.504 | 1.00 | 36.24  |
|    | ATOM | 154 | N   | HIS | A | 22 | -1.110 | 40.475 | 45.203 | 1.00 | 28.25  |
|    | ATOM | 155 | CA  | HIS | A | 22 | -0.852 | 41.482 | 44.186 | 1.00 | 30.03  |
| 35 | ATOM | 156 | C   | HIS | A | 22 | -1.272 | 42.800 | 44.795 | 1.00 | 31.36  |
|    | ATOM | 157 | O   | HIS | A | 22 | -2.435 | 42.993 | 45.127 | 1.00 | 30.57  |
|    | ATOM | 158 | CB  | HIS | A | 22 | -1.560 | 41.291 | 42.844 | 1.00 | 31.66  |
|    | ATOM | 159 | CG  | HIS | A | 22 | -1.060 | 42.347 | 41.913 | 1.00 | 34.36  |
|    | ATOM | 160 | ND1 | HIS | A | 22 | -1.913 | 43.134 | 41.187 | 1.00 | 37.39  |
| 40 | ATOM | 161 | CD2 | HIS | A | 22 | 0.208  | 42.734 | 41.635 | 1.00 | 37.45  |
|    | ATOM | 162 | CE1 | HIS | A | 22 | -1.155 | 43.968 | 40.481 | 1.00 | 38.02  |
|    | ATOM | 163 | NE2 | HIS | A | 22 | 0.132  | 43.757 | 40.730 | 1.00 | 37.95  |
|    | ATOM | 164 | N   | LEU | A | 23 | -0.315 | 43.668 | 45.000 | 1.00 | 31.07  |
|    | ATOM | 165 | CA  | LEU | A | 23 | -0.593 | 44.939 | 45.637 | 1.00 | 31.63  |
| 45 | ATOM | 166 | C   | LEU | A | 23 | -0.469 | 46.144 | 44.705 | 1.00 | 32.72  |
|    | ATOM | 167 | O   | LEU | A | 23 | 0.563  | 46.431 | 44.093 | 1.00 | 34.74  |
|    | ATOM | 168 | CB  | LEU | A | 23 | 0.299  | 45.093 | 46.894 | 1.00 | 31.20  |
|    | ATOM | 169 | CG  | LEU | A | 23 | -0.320 | 45.795 | 48.126 | 1.00 | 34.26  |
|    | ATOM | 170 | CD1 | LEU | A | 23 | 0.543  | 46.966 | 48.510 | 1.00 | 32.64  |
| 50 | ATOM | 171 | CD2 | LEU | A | 23 | -1.759 | 46.263 | 47.957 | 1.00 | 34.32  |
|    | ATOM | 172 | N   | ARG | A | 24 | -1.576 | 46.840 | 44.623 | 1.00 | 28.33  |
|    | ATOM | 173 | CA  | ARG | A | 24 | -1.681 | 48.040 | 43.837 | 1.00 | 30.28  |
|    | ATOM | 174 | C   | ARG | A | 24 | -2.162 | 49.119 | 44.794 | 1.00 | 35.16  |
|    | ATOM | 175 | O   | ARG | A | 24 | -3.251 | 49.005 | 45.349 | 1.00 | 35.74  |
| 55 | ATOM | 176 | CB  | ARG | A | 24 | -2.651 | 47.860 | 42.689 | 1.00 | 32.69  |
|    | ATOM | 177 | CG  | ARG | A | 24 | -1.962 | 47.363 | 41.423 | 1.00 | 55.58  |
|    | ATOM | 178 | CD  | ARG | A | 24 | -2.732 | 47.698 | 40.144 | 1.00 | 67.44  |
|    | ATOM | 179 | NE  | ARG | A | 24 | -3.993 | 46.971 | 40.030 | 1.00 | 64.57  |
|    | ATOM | 180 | CZ  | ARG | A | 24 | -5.150 | 47.440 | 40.498 | 1.00 | 97.41  |
| 60 | ATOM | 181 | NH1 | ARG | A | 24 | -5.246 | 48.624 | 41.108 | 1.00 | 81.55  |
|    | ATOM | 182 | NH2 | ARG | A | 24 | -6.249 | 46.713 | 40.344 | 1.00 | 100.00 |
|    | ATOM | 183 | N   | CYS | A | 25 | -1.320 | 50.126 | 45.045 | 1.00 | 36.40  |
|    | ATOM | 184 | CA  | CYS | A | 25 | -1.696 | 51.181 | 45.998 | 1.00 | 36.70  |
|    | ATOM | 185 | C   | CYS | A | 25 | -0.996 | 52.522 | 45.815 | 1.00 | 34.57  |
|    | ATOM | 186 | O   | CYS | A | 25 | 0.030  | 52.676 | 45.100 | 1.00 | 30.46  |



|    |      |     |     |     |   |    |        |        |        |      |       |
|----|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|
|    | ATOM | 187 | CB  | CYS | A | 25 | -1.599 | 50.732 | 47.481 | 1.00 | 37.45 |
|    | ATOM | 188 | SG  | CYS | A | 25 | 0.119  | 50.641 | 48.047 | 1.00 | 41.07 |
|    | ATOM | 189 | N   | SER | A | 26 | -1.606 | 53.493 | 46.507 | 1.00 | 32.19 |
| 5  | ATOM | 190 | CA  | SER | A | 26 | -1.098 | 54.841 | 46.486 | 1.00 | 32.91 |
|    | ATOM | 191 | C   | SER | A | 26 | -0.861 | 55.372 | 47.877 | 1.00 | 28.73 |
|    | ATOM | 192 | O   | SER | A | 26 | -1.638 | 55.107 | 48.802 | 1.00 | 24.93 |
|    | ATOM | 193 | CB  | SER | A | 26 | -1.884 | 55.825 | 45.626 | 1.00 | 41.21 |
|    | ATOM | 194 | OG  | SER | A | 26 | -0.987 | 56.748 | 45.012 | 1.00 | 55.61 |
| 10 | ATOM | 195 | N   | VAL | A | 27 | 0.258  | 56.092 | 47.964 | 1.00 | 28.06 |
|    | ATOM | 196 | CA  | VAL | A | 27 | 0.719  | 56.718 | 49.172 | 1.00 | 29.85 |
|    | ATOM | 197 | C   | VAL | A | 27 | 0.330  | 58.199 | 49.211 | 1.00 | 33.50 |
|    | ATOM | 198 | O   | VAL | A | 27 | 0.868  | 59.024 | 48.443 | 1.00 | 31.85 |
|    | ATOM | 199 | CB  | VAL | A | 27 | 2.217  | 56.509 | 49.370 | 1.00 | 34.37 |
|    | ATOM | 200 | CG1 | VAL | A | 27 | 2.605  | 57.003 | 50.774 | 1.00 | 35.81 |
| 15 | ATOM | 201 | CG2 | VAL | A | 27 | 2.481  | 55.004 | 49.263 | 1.00 | 33.03 |
|    | ATOM | 202 | N   | ASP | A | 28 | -0.626 | 58.489 | 50.106 | 1.00 | 31.46 |
|    | ATOM | 203 | CA  | ASP | A | 28 | -1.137 | 59.841 | 50.327 | 1.00 | 32.29 |
|    | ATOM | 204 | C   | ASP | A | 28 | -0.700 | 60.403 | 51.687 | 1.00 | 27.74 |
| 20 | ATOM | 205 | O   | ASP | A | 28 | -1.254 | 60.057 | 52.728 | 1.00 | 25.85 |
|    | ATOM | 206 | CB  | ASP | A | 28 | -2.663 | 59.943 | 50.144 | 1.00 | 35.45 |
|    | ATOM | 207 | CG  | ASP | A | 28 | -3.158 | 61.380 | 50.016 | 1.00 | 43.54 |
|    | ATOM | 208 | OD1 | ASP | A | 28 | -2.559 | 62.348 | 50.463 | 1.00 | 39.89 |
|    | ATOM | 209 | OD2 | ASP | A | 28 | -4.290 | 61.467 | 49.353 | 1.00 | 50.90 |
| 25 | ATOM | 210 | N   | PHE | A | 29 | 0.311  | 61.251 | 51.614 | 1.00 | 29.04 |
|    | ATOM | 211 | CA  | PHE | A | 29 | 0.913  | 61.918 | 52.741 | 1.00 | 32.69 |
|    | ATOM | 212 | C   | PHE | A | 29 | 0.011  | 63.004 | 53.317 | 1.00 | 46.23 |
|    | ATOM | 213 | O   | PHE | A | 29 | 0.021  | 63.341 | 54.511 | 1.00 | 49.95 |
|    | ATOM | 214 | CB  | PHE | A | 29 | 2.199  | 62.568 | 52.288 | 1.00 | 34.84 |
| 30 | ATOM | 215 | CG  | PHE | A | 29 | 3.371  | 61.627 | 52.322 | 1.00 | 37.91 |
|    | ATOM | 216 | CD1 | PHE | A | 29 | 3.961  | 61.270 | 53.534 | 1.00 | 39.04 |
|    | ATOM | 217 | CD2 | PHE | A | 29 | 3.893  | 61.111 | 51.136 | 1.00 | 39.45 |
|    | ATOM | 218 | CE1 | PHE | A | 29 | 5.064  | 60.419 | 53.565 | 1.00 | 39.96 |
|    | ATOM | 219 | CE2 | PHE | A | 29 | 4.992  | 60.254 | 51.153 | 1.00 | 43.33 |
| 35 | ATOM | 220 | CZ  | PHE | A | 29 | 5.573  | 59.908 | 52.373 | 1.00 | 39.81 |
|    | ATOM | 221 | N   | THR | A | 30 | -0.788 | 63.569 | 52.445 | 1.00 | 43.44 |
|    | ATOM | 222 | CA  | THR | A | 30 | -1.695 | 64.590 | 52.870 | 1.00 | 40.68 |
|    | ATOM | 223 | C   | THR | A | 30 | -2.776 | 63.990 | 53.751 | 1.00 | 36.25 |
|    | ATOM | 224 | O   | THR | A | 30 | -3.160 | 64.575 | 54.741 | 1.00 | 37.59 |
| 40 | ATOM | 225 | CB  | THR | A | 30 | -2.241 | 65.353 | 51.661 | 1.00 | 44.14 |
|    | ATOM | 226 | OG1 | THR | A | 30 | -1.312 | 66.379 | 51.280 | 1.00 | 35.00 |
|    | ATOM | 227 | CG2 | THR | A | 30 | -3.634 | 65.886 | 51.979 | 1.00 | 42.00 |
|    | ATOM | 228 | N   | ARG | A | 31 | -3.249 | 62.803 | 53.426 | 1.00 | 23.27 |
|    | ATOM | 229 | CA  | ARG | A | 31 | -4.258 | 62.179 | 54.263 | 1.00 | 22.52 |
| 45 | ATOM | 230 | C   | ARG | A | 31 | -3.670 | 61.084 | 55.187 | 1.00 | 28.33 |
|    | ATOM | 231 | O   | ARG | A | 31 | -4.388 | 60.485 | 56.013 | 1.00 | 26.36 |
|    | ATOM | 232 | CB  | ARG | A | 31 | -5.360 | 61.545 | 53.423 | 1.00 | 29.16 |
|    | ATOM | 233 | CG  | ARG | A | 31 | -6.236 | 62.579 | 52.723 | 1.00 | 52.89 |
|    | ATOM | 234 | CD  | ARG | A | 31 | -6.324 | 62.368 | 51.215 | 1.00 | 63.14 |
| 50 | ATOM | 235 | NE  | ARG | A | 31 | -5.912 | 63.537 | 50.434 | 1.00 | 56.84 |
|    | ATOM | 236 | CZ  | ARG | A | 31 | -6.777 | 64.353 | 49.868 | 1.00 | 58.33 |
|    | ATOM | 237 | NH1 | ARG | A | 31 | -8.084 | 64.154 | 49.996 | 1.00 | 45.96 |
|    | ATOM | 238 | NH2 | ARG | A | 31 | -6.335 | 65.393 | 49.166 | 1.00 | 57.96 |
|    | ATOM | 239 | N   | ARG | A | 32 | -2.353 | 60.838 | 55.018 | 1.00 | 28.39 |
| 55 | ATOM | 240 | CA  | ARG | A | 32 | -1.587 | 59.832 | 55.754 | 1.00 | 28.42 |
|    | ATOM | 241 | C   | ARG | A | 32 | -2.248 | 58.498 | 55.548 | 1.00 | 31.13 |
|    | ATOM | 242 | O   | ARG | A | 32 | -2.553 | 57.754 | 56.484 | 1.00 | 26.52 |
|    | ATOM | 243 | CB  | ARG | A | 32 | -1.353 | 60.163 | 57.233 | 1.00 | 22.96 |
|    | ATOM | 244 | CG  | ARG | A | 32 | -1.083 | 61.654 | 57.442 | 1.00 | 46.47 |
| 60 | ATOM | 245 | CD  | ARG | A | 32 | 0.247  | 62.022 | 58.108 | 1.00 | 65.92 |
|    | ATOM | 246 | NE  | ARG | A | 32 | 0.307  | 61.670 | 59.532 | 1.00 | 62.95 |
|    | ATOM | 247 | CZ  | ARG | A | 32 | 1.244  | 62.060 | 60.403 | 1.00 | 56.24 |
|    | ATOM | 248 | NH1 | ARG | A | 32 | 2.259  | 62.862 | 60.090 | 1.00 | 38.45 |
|    | ATOM | 249 | NH2 | ARG | A | 32 | 1.150  | 61.628 | 61.644 | 1.00 | 38.26 |
|    | ATOM | 250 | N   | THR | A | 33 | -2.503 | 58.222 | 54.278 | 1.00 | 30.15 |



|    |      |     |     |     |   |    |        |        |        |      |       |
|----|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|
|    | ATOM | 251 | CA  | THR | A | 33 | -3.148 | 56.969 | 53.940 | 1.00 | 30.69 |
|    | ATOM | 252 | C   | THR | A | 33 | -2.460 | 56.247 | 52.816 | 1.00 | 30.70 |
|    | ATOM | 253 | O   | THR | A | 33 | -1.765 | 56.842 | 51.978 | 1.00 | 27.23 |
| 5  | ATOM | 254 | CB  | THR | A | 33 | -4.603 | 57.146 | 53.467 | 1.00 | 39.23 |
|    | ATOM | 255 | OG1 | THR | A | 33 | -4.637 | 58.100 | 52.420 | 1.00 | 37.97 |
|    | ATOM | 256 | CG2 | THR | A | 33 | -5.567 | 57.481 | 54.598 | 1.00 | 34.16 |
|    | ATOM | 257 | N   | LEU | A | 34 | -2.719 | 54.950 | 52.842 | 1.00 | 30.87 |
|    | ATOM | 258 | CA  | LEU | A | 34 | -2.279 | 54.012 | 51.842 | 1.00 | 32.01 |
| 10 | ATOM | 259 | C   | LEU | A | 34 | -3.598 | 53.483 | 51.332 | 1.00 | 26.54 |
|    | ATOM | 260 | O   | LEU | A | 34 | -4.426 | 53.031 | 52.106 | 1.00 | 25.08 |
|    | ATOM | 261 | CB  | LEU | A | 34 | -1.518 | 52.805 | 52.428 | 1.00 | 35.05 |
|    | ATOM | 262 | CG  | LEU | A | 34 | -0.007 | 52.880 | 52.357 | 1.00 | 42.66 |
|    | ATOM | 263 | CD1 | LEU | A | 34 | 0.537  | 51.446 | 52.425 | 1.00 | 41.75 |
|    | ATOM | 264 | CD2 | LEU | A | 34 | 0.434  | 53.610 | 51.081 | 1.00 | 49.07 |
| 15 | ATOM | 265 | N   | THR | A | 35 | -3.828 | 53.576 | 50.050 | 1.00 | 27.44 |
|    | ATOM | 266 | CA  | THR | A | 35 | -5.088 | 53.081 | 49.552 | 1.00 | 29.43 |
|    | ATOM | 267 | C   | THR | A | 35 | -4.825 | 52.257 | 48.316 | 1.00 | 33.69 |
|    | ATOM | 268 | O   | THR | A | 35 | -3.896 | 52.559 | 47.532 | 1.00 | 31.06 |
|    | ATOM | 269 | CB  | THR | A | 35 | -6.004 | 54.248 | 49.195 | 1.00 | 49.67 |
| 20 | ATOM | 270 | OG1 | THR | A | 35 | -5.775 | 55.297 | 50.111 | 1.00 | 56.12 |
|    | ATOM | 271 | CG2 | THR | A | 35 | -7.442 | 53.781 | 49.282 | 1.00 | 53.32 |
|    | ATOM | 272 | N   | GLY | A | 36 | -5.638 | 51.220 | 48.172 | 1.00 | 31.25 |
|    | ATOM | 273 | CA  | GLY | A | 36 | -5.509 | 50.336 | 47.024 | 1.00 | 30.78 |
|    | ATOM | 274 | C   | GLY | A | 36 | -6.314 | 49.072 | 47.144 | 1.00 | 27.36 |
| 25 | ATOM | 275 | O   | GLY | A | 36 | -7.358 | 48.969 | 47.773 | 1.00 | 26.53 |
|    | ATOM | 276 | N   | THR | A | 37 | -5.809 | 48.080 | 46.504 | 1.00 | 27.32 |
|    | ATOM | 277 | CA  | THR | A | 37 | -6.478 | 46.793 | 46.579 | 1.00 | 29.08 |
|    | ATOM | 278 | C   | THR | A | 37 | -5.460 | 45.717 | 46.846 | 1.00 | 29.62 |
|    | ATOM | 279 | O   | THR | A | 37 | -4.321 | 45.787 | 46.370 | 1.00 | 27.85 |
| 30 | ATOM | 280 | CB  | THR | A | 37 | -7.268 | 46.425 | 45.311 | 1.00 | 35.94 |
|    | ATOM | 281 | OG1 | THR | A | 37 | -6.546 | 46.790 | 44.142 | 1.00 | 33.45 |
|    | ATOM | 282 | CG2 | THR | A | 37 | -8.601 | 47.144 | 45.350 | 1.00 | 41.23 |
|    | ATOM | 283 | N   | ALA | A | 38 | -5.867 | 44.738 | 47.609 | 1.00 | 28.10 |
|    | ATOM | 284 | CA  | ALA | A | 38 | -4.934 | 43.674 | 47.856 | 1.00 | 27.55 |
| 35 | ATOM | 285 | C   | ALA | A | 38 | -5.482 | 42.447 | 47.137 | 1.00 | 30.70 |
|    | ATOM | 286 | O   | ALA | A | 38 | -6.536 | 41.941 | 47.510 | 1.00 | 31.51 |
|    | ATOM | 287 | CB  | ALA | A | 38 | -4.803 | 43.425 | 49.339 | 1.00 | 26.00 |
|    | ATOM | 288 | N   | ALA | A | 39 | -4.798 | 41.981 | 46.090 | 1.00 | 27.63 |
|    | ATOM | 289 | CA  | ALA | A | 39 | -5.280 | 40.761 | 45.394 | 1.00 | 29.40 |
| 40 | ATOM | 290 | C   | ALA | A | 39 | -4.563 | 39.541 | 45.966 | 1.00 | 29.05 |
|    | ATOM | 291 | O   | ALA | A | 39 | -3.371 | 39.333 | 45.734 | 1.00 | 28.04 |
|    | ATOM | 292 | CB  | ALA | A | 39 | -5.024 | 40.787 | 43.888 | 1.00 | 30.14 |
|    | ATOM | 293 | N   | LEU | A | 40 | -5.327 | 38.780 | 46.713 | 1.00 | 26.03 |
|    | ATOM | 294 | CA  | LEU | A | 40 | -4.899 | 37.591 | 47.392 | 1.00 | 26.04 |
| 45 | ATOM | 295 | C   | LEU | A | 40 | -5.304 | 36.310 | 46.637 | 1.00 | 30.62 |
|    | ATOM | 296 | O   | LEU | A | 40 | -6.499 | 36.038 | 46.394 | 1.00 | 28.36 |
|    | ATOM | 297 | CB  | LEU | A | 40 | -5.596 | 37.499 | 48.779 | 1.00 | 24.92 |
|    | ATOM | 298 | CG  | LEU | A | 40 | -5.312 | 38.663 | 49.725 | 1.00 | 27.54 |
|    | ATOM | 299 | CD1 | LEU | A | 40 | -5.870 | 38.272 | 51.074 | 1.00 | 29.18 |
| 50 | ATOM | 300 | CD2 | LEU | A | 40 | -3.817 | 38.865 | 49.857 | 1.00 | 26.20 |
|    | ATOM | 301 | N   | THR | A | 41 | -4.302 | 35.498 | 46.326 | 1.00 | 23.66 |
|    | ATOM | 302 | CA  | THR | A | 41 | -4.566 | 34.232 | 45.700 | 1.00 | 23.84 |
|    | ATOM | 303 | C   | THR | A | 41 | -4.509 | 33.259 | 46.841 | 1.00 | 28.24 |
|    | ATOM | 304 | O   | THR | A | 41 | -3.448 | 33.076 | 47.421 | 1.00 | 28.49 |
| 55 | ATOM | 305 | CB  | THR | A | 41 | -3.554 | 33.854 | 44.613 | 1.00 | 38.89 |
|    | ATOM | 306 | OG1 | THR | A | 41 | -3.594 | 34.801 | 43.555 | 1.00 | 32.11 |
|    | ATOM | 307 | CG2 | THR | A | 41 | -3.856 | 32.426 | 44.113 | 1.00 | 33.97 |
|    | ATOM | 308 | N   | VAL | A | 42 | -5.674 | 32.704 | 47.169 | 1.00 | 25.76 |
|    | ATOM | 309 | CA  | VAL | A | 42 | -5.843 | 31.782 | 48.261 | 1.00 | 26.45 |
| 60 | ATOM | 310 | C   | VAL | A | 42 | -6.068 | 30.356 | 47.804 | 1.00 | 34.04 |
|    | ATOM | 311 | O   | VAL | A | 42 | -6.730 | 30.118 | 46.795 | 1.00 | 33.15 |
|    | ATOM | 312 | CB  | VAL | A | 42 | -7.024 | 32.223 | 49.113 | 1.00 | 29.66 |
|    | ATOM | 313 | CG1 | VAL | A | 42 | -7.189 | 31.274 | 50.295 | 1.00 | 30.14 |
|    | ATOM | 314 | CG2 | VAL | A | 42 | -6.805 | 33.657 | 49.611 | 1.00 | 28.98 |



|    |      |     |     |     |   |    |         |        |        |      |        |
|----|------|-----|-----|-----|---|----|---------|--------|--------|------|--------|
|    | ATOM | 315 | N   | GLN | A | 43 | -5.530  | 29.405 | 48.566 | 1.00 | 29.23  |
|    | ATOM | 316 | CA  | GLN | A | 43 | -5.692  | 27.989 | 48.247 | 1.00 | 28.15  |
|    | ATOM | 317 | C   | GLN | A | 43 | -6.357  | 27.171 | 49.356 | 1.00 | 31.60  |
| 5  | ATOM | 318 | O   | GLN | A | 43 | -5.916  | 27.081 | 50.506 | 1.00 | 30.09  |
|    | ATOM | 319 | CB  | GLN | A | 43 | -4.401  | 27.337 | 47.748 | 1.00 | 29.76  |
|    | ATOM | 320 | CG  | GLN | A | 43 | -4.305  | 25.877 | 48.214 | 1.00 | 49.25  |
|    | ATOM | 321 | CD  | GLN | A | 43 | -2.920  | 25.308 | 48.018 | 1.00 | 68.40  |
|    | ATOM | 322 | OE1 | GLN | A | 43 | -2.508  | 25.059 | 46.882 | 1.00 | 65.93  |
| 10 | ATOM | 323 | NE2 | GLN | A | 43 | -2.190  | 25.118 | 49.116 | 1.00 | 62.52  |
|    | ATOM | 324 | N   | SER | A | 44 | -7.470  | 26.553 | 49.027 | 1.00 | 25.74  |
|    | ATOM | 325 | CA  | SER | A | 44 | -8.159  | 25.793 | 50.027 | 1.00 | 24.21  |
|    | ATOM | 326 | C   | SER | A | 44 | -7.406  | 24.562 | 50.434 | 1.00 | 31.27  |
|    | ATOM | 327 | O   | SER | A | 44 | -6.701  | 23.950 | 49.642 | 1.00 | 33.21  |
| 15 | ATOM | 328 | CB  | SER | A | 44 | -9.542  | 25.400 | 49.574 | 1.00 | 28.22  |
|    | ATOM | 329 | OG  | SER | A | 44 | -10.143 | 24.569 | 50.550 | 1.00 | 36.23  |
|    | ATOM | 330 | N   | GLN | A | 45 | -7.593  | 24.190 | 51.685 | 1.00 | 29.25  |
|    | ATOM | 331 | CA  | GLN | A | 45 | -6.964  | 23.016 | 52.240 | 1.00 | 32.48  |
|    | ATOM | 332 | C   | GLN | A | 45 | -8.027  | 22.007 | 52.618 | 1.00 | 41.18  |
| 20 | ATOM | 333 | O   | GLN | A | 45 | -7.757  | 20.936 | 53.165 | 1.00 | 37.68  |
|    | ATOM | 334 | CB  | GLN | A | 45 | -6.095  | 23.387 | 53.451 | 1.00 | 35.17  |
|    | ATOM | 335 | CG  | GLN | A | 45 | -5.138  | 24.525 | 53.090 | 1.00 | 29.17  |
|    | ATOM | 336 | CD  | GLN | A | 45 | -4.197  | 24.179 | 51.954 | 1.00 | 37.50  |
|    | ATOM | 337 | OE1 | GLN | A | 45 | -4.107  | 24.903 | 50.939 | 1.00 | 44.48  |
| 25 | ATOM | 338 | NE2 | GLN | A | 45 | -3.466  | 23.083 | 52.127 | 1.00 | 23.35  |
|    | ATOM | 339 | N   | GLU | A | 46 | -9.258  | 22.387 | 52.322 | 1.00 | 40.69  |
|    | ATOM | 340 | CA  | GLU | A | 46 | -10.391 | 21.548 | 52.591 | 1.00 | 41.85  |
|    | ATOM | 341 | C   | GLU | A | 46 | -11.311 | 21.472 | 51.388 | 1.00 | 46.94  |
|    | ATOM | 342 | O   | GLU | A | 46 | -11.146 | 22.143 | 50.367 | 1.00 | 45.45  |
| 30 | ATOM | 343 | CB  | GLU | A | 46 | -11.216 | 21.989 | 53.827 | 1.00 | 42.82  |
|    | ATOM | 344 | CG  | GLU | A | 46 | -10.736 | 23.256 | 54.548 | 1.00 | 48.14  |
|    | ATOM | 345 | CD  | GLU | A | 46 | -11.469 | 23.463 | 55.856 | 1.00 | 62.06  |
|    | ATOM | 346 | OE1 | GLU | A | 46 | -12.507 | 24.103 | 55.957 | 1.00 | 64.38  |
|    | ATOM | 347 | OE2 | GLU | A | 46 | -10.880 | 22.875 | 56.871 | 1.00 | 51.57  |
| 35 | ATOM | 348 | N   | ASP | A | 47 | -12.306 | 20.638 | 51.523 | 1.00 | 46.70  |
|    | ATOM | 349 | CA  | ASP | A | 47 | -13.261 | 20.543 | 50.464 | 1.00 | 48.51  |
|    | ATOM | 350 | C   | ASP | A | 47 | -14.408 | 21.358 | 50.947 | 1.00 | 45.90  |
|    | ATOM | 351 | O   | ASP | A | 47 | -14.674 | 21.368 | 52.148 | 1.00 | 41.55  |
|    | ATOM | 352 | CB  | ASP | A | 47 | -13.748 | 19.104 | 50.220 | 1.00 | 52.32  |
| 40 | ATOM | 353 | CG  | ASP | A | 47 | -12.739 | 18.258 | 49.495 | 1.00 | 80.62  |
|    | ATOM | 354 | OD1 | ASP | A | 47 | -12.338 | 18.505 | 48.364 | 1.00 | 77.22  |
|    | ATOM | 355 | OD2 | ASP | A | 47 | -12.330 | 17.237 | 50.218 | 1.00 | 100.00 |
|    | ATOM | 356 | N   | ASN | A | 48 | -15.067 | 22.044 | 50.045 | 1.00 | 44.45  |
|    | ATOM | 357 | CA  | ASN | A | 48 | -16.209 | 22.826 | 50.475 | 1.00 | 45.83  |
| 45 | ATOM | 358 | C   | ASN | A | 48 | -15.875 | 24.055 | 51.308 | 1.00 | 46.95  |
|    | ATOM | 359 | O   | ASN | A | 48 | -16.620 | 24.449 | 52.219 | 1.00 | 45.85  |
|    | ATOM | 360 | CB  | ASN | A | 48 | -17.246 | 21.959 | 51.225 | 1.00 | 43.60  |
|    | ATOM | 361 | CG  | ASN | A | 48 | -18.653 | 22.469 | 51.004 | 1.00 | 65.69  |
|    | ATOM | 362 | OD1 | ASN | A | 48 | -18.924 | 23.191 | 50.027 | 1.00 | 68.02  |
| 50 | ATOM | 363 | ND2 | ASN | A | 48 | -19.545 | 22.123 | 51.922 | 1.00 | 53.94  |
|    | ATOM | 364 | N   | LEU | A | 49 | -14.758 | 24.672 | 51.004 | 1.00 | 40.04  |
|    | ATOM | 365 | CA  | LEU | A | 49 | -14.445 | 25.850 | 51.741 | 1.00 | 35.92  |
|    | ATOM | 366 | C   | LEU | A | 49 | -15.377 | 26.909 | 51.178 | 1.00 | 39.46  |
|    | ATOM | 367 | O   | LEU | A | 49 | -15.301 | 27.241 | 49.998 | 1.00 | 36.67  |
| 55 | ATOM | 368 | CB  | LEU | A | 49 | -12.977 | 26.218 | 51.556 | 1.00 | 34.20  |
|    | ATOM | 369 | CG  | LEU | A | 49 | -12.623 | 27.492 | 52.307 | 1.00 | 36.68  |
|    | ATOM | 370 | CD1 | LEU | A | 49 | -13.000 | 27.286 | 53.753 | 1.00 | 35.00  |
|    | ATOM | 371 | CD2 | LEU | A | 49 | -11.135 | 27.785 | 52.181 | 1.00 | 38.84  |
|    | ATOM | 372 | N   | ARG | A | 50 | -16.287 | 27.411 | 51.998 | 1.00 | 40.21  |
| 60 | ATOM | 373 | CA  | ARG | A | 50 | -17.242 | 28.417 | 51.525 | 1.00 | 41.40  |
|    | ATOM | 374 | C   | ARG | A | 50 | -16.907 | 29.859 | 51.901 | 1.00 | 47.29  |
|    | ATOM | 375 | O   | ARG | A | 50 | -17.364 | 30.801 | 51.263 | 1.00 | 47.10  |
|    | ATOM | 376 | CB  | ARG | A | 50 | -18.644 | 28.046 | 51.980 | 1.00 | 38.23  |
|    | ATOM | 377 | CG  | ARG | A | 50 | -18.911 | 26.547 | 51.811 | 1.00 | 52.44  |
|    | ATOM | 378 | CD  | ARG | A | 50 | -20.385 | 26.171 | 51.839 | 1.00 | 58.37  |



|    |      |     |     |     |   |    |         |        |        |      |        |
|----|------|-----|-----|-----|---|----|---------|--------|--------|------|--------|
|    | ATOM | 379 | NE  | ARG | A | 50 | -20.835 | 25.461 | 50.643 | 1.00 | 80.87  |
|    | ATOM | 380 | CZ  | ARG | A | 50 | -21.951 | 24.727 | 50.592 | 1.00 | 100.00 |
|    | ATOM | 381 | NH1 | ARG | A | 50 | -22.750 | 24.575 | 51.652 | 1.00 | 100.00 |
| 5  | ATOM | 382 | NH2 | ARG | A | 50 | -22.272 | 24.127 | 49.446 | 1.00 | 65.83  |
|    | ATOM | 383 | N   | SER | A | 51 | -16.102 | 30.024 | 52.945 | 1.00 | 43.64  |
|    | ATOM | 384 | CA  | SER | A | 51 | -15.714 | 31.334 | 53.418 | 1.00 | 41.14  |
|    | ATOM | 385 | C   | SER | A | 51 | -14.454 | 31.283 | 54.259 | 1.00 | 44.29  |
|    | ATOM | 386 | O   | SER | A | 51 | -14.253 | 30.319 | 55.016 | 1.00 | 46.38  |
| 10 | ATOM | 387 | CB  | SER | A | 51 | -16.821 | 31.863 | 54.321 | 1.00 | 45.40  |
|    | ATOM | 388 | OG  | SER | A | 51 | -16.862 | 31.143 | 55.556 | 1.00 | 46.27  |
|    | ATOM | 389 | N   | LEU | A | 52 | -13.623 | 32.330 | 54.156 | 1.00 | 36.51  |
|    | ATOM | 390 | CA  | LEU | A | 52 | -12.418 | 32.411 | 54.964 | 1.00 | 36.39  |
|    | ATOM | 391 | C   | LEU | A | 52 | -12.369 | 33.667 | 55.852 | 1.00 | 42.80  |
| 15 | ATOM | 392 | O   | LEU | A | 52 | -13.113 | 34.644 | 55.647 | 1.00 | 40.92  |
|    | ATOM | 393 | CB  | LEU | A | 52 | -11.103 | 32.143 | 54.203 | 1.00 | 35.84  |
|    | ATOM | 394 | CG  | LEU | A | 52 | -10.729 | 33.115 | 53.095 | 1.00 | 39.41  |
|    | ATOM | 395 | CD1 | LEU | A | 52 | -11.745 | 33.042 | 51.994 | 1.00 | 41.33  |
|    | ATOM | 396 | CD2 | LEU | A | 52 | -10.624 | 34.538 | 53.605 | 1.00 | 38.19  |
| 20 | ATOM | 397 | N   | VAL | A | 53 | -11.491 | 33.659 | 56.859 | 1.00 | 37.98  |
|    | ATOM | 398 | CA  | VAL | A | 53 | -11.331 | 34.834 | 57.737 | 1.00 | 34.43  |
|    | ATOM | 399 | C   | VAL | A | 53 | -9.933  | 35.384 | 57.550 | 1.00 | 31.66  |
|    | ATOM | 400 | O   | VAL | A | 53 | -8.975  | 34.606 | 57.511 | 1.00 | 28.02  |
|    | ATOM | 401 | CB  | VAL | A | 53 | -11.601 | 34.597 | 59.226 | 1.00 | 37.95  |
| 25 | ATOM | 402 | CG1 | VAL | A | 53 | -11.580 | 35.929 | 59.989 | 1.00 | 37.38  |
|    | ATOM | 403 | CG2 | VAL | A | 53 | -12.946 | 33.922 | 59.419 | 1.00 | 37.84  |
|    | ATOM | 404 | N   | LEU | A | 54 | -9.829  | 36.705 | 57.418 | 1.00 | 23.95  |
|    | ATOM | 405 | CA  | LEU | A | 54 | -8.558  | 37.365 | 57.270 | 1.00 | 22.89  |
|    | ATOM | 406 | C   | LEU | A | 54 | -8.395  | 38.285 | 58.470 | 1.00 | 29.33  |
| 30 | ATOM | 407 | O   | LEU | A | 54 | -9.388  | 38.613 | 59.138 | 1.00 | 25.65  |
|    | ATOM | 408 | CB  | LEU | A | 54 | -8.515  | 38.242 | 56.019 | 1.00 | 23.57  |
|    | ATOM | 409 | CG  | LEU | A | 54 | -8.458  | 37.469 | 54.700 | 1.00 | 32.01  |
|    | ATOM | 410 | CD1 | LEU | A | 54 | -8.345  | 38.475 | 53.541 | 1.00 | 31.66  |
|    | ATOM | 411 | CD2 | LEU | A | 54 | -7.271  | 36.505 | 54.684 | 1.00 | 24.96  |
| 35 | ATOM | 412 | N   | ASP | A | 55 | -7.145  | 38.698 | 58.732 | 1.00 | 28.72  |
|    | ATOM | 413 | CA  | ASP | A | 55 | -6.830  | 39.616 | 59.831 | 1.00 | 24.54  |
|    | ATOM | 414 | C   | ASP | A | 55 | -6.845  | 41.043 | 59.289 | 1.00 | 22.50  |
|    | ATOM | 415 | O   | ASP | A | 55 | -6.460  | 41.312 | 58.173 | 1.00 | 21.41  |
|    | ATOM | 416 | CB  | ASP | A | 55 | -5.446  | 39.344 | 60.500 | 1.00 | 25.99  |
| 40 | ATOM | 417 | CG  | ASP | A | 55 | -5.298  | 38.132 | 61.418 | 1.00 | 23.16  |
|    | ATOM | 418 | OD1 | ASP | A | 55 | -5.887  | 37.985 | 62.470 | 1.00 | 27.99  |
|    | ATOM | 419 | OD2 | ASP | A | 55 | -4.408  | 37.248 | 60.991 | 1.00 | 24.58  |
|    | ATOM | 420 | N   | THR | A | 56 | -7.309  | 41.977 | 60.109 | 1.00 | 21.37  |
|    | ATOM | 421 | CA  | THR | A | 56 | -7.346  | 43.373 | 59.748 | 1.00 | 22.34  |
| 45 | ATOM | 422 | C   | THR | A | 56 | -7.167  | 44.196 | 61.019 | 1.00 | 25.71  |
|    | ATOM | 423 | O   | THR | A | 56 | -7.573  | 43.726 | 62.088 | 1.00 | 26.22  |
|    | ATOM | 424 | CB  | THR | A | 56 | -8.727  | 43.717 | 59.133 | 1.00 | 34.75  |
|    | ATOM | 425 | OG1 | THR | A | 56 | -9.668  | 43.936 | 60.183 | 1.00 | 35.02  |
|    | ATOM | 426 | CG2 | THR | A | 56 | -9.210  | 42.578 | 58.241 | 1.00 | 40.12  |
| 50 | ATOM | 427 | N   | LYS | A | 57 | -6.598  | 45.405 | 60.918 | 1.00 | 20.41  |
|    | ATOM | 428 | CA  | LYS | A | 57 | -6.478  | 46.239 | 62.114 | 1.00 | 19.63  |
|    | ATOM | 429 | C   | LYS | A | 57 | -6.656  | 47.686 | 61.717 | 1.00 | 21.21  |
|    | ATOM | 430 | O   | LYS | A | 57 | -5.851  | 48.222 | 60.995 | 1.00 | 19.18  |
|    | ATOM | 431 | CB  | LYS | A | 57 | -5.182  | 45.983 | 62.827 | 1.00 | 21.05  |
| 55 | ATOM | 432 | CG  | LYS | A | 57 | -5.137  | 46.424 | 64.271 | 1.00 | 26.38  |
|    | ATOM | 433 | CD  | LYS | A | 57 | -3.713  | 46.855 | 64.626 | 1.00 | 44.32  |
|    | ATOM | 434 | CE  | LYS | A | 57 | -3.331  | 46.750 | 66.099 | 1.00 | 61.77  |
|    | ATOM | 435 | NZ  | LYS | A | 57 | -1.996  | 47.313 | 66.396 | 1.00 | 53.68  |
|    | ATOM | 436 | N   | ASP | A | 58 | -7.739  | 48.322 | 62.162 | 1.00 | 23.32  |
| 60 | ATOM | 437 | CA  | ASP | A | 58 | -7.952  | 49.707 | 61.772 | 1.00 | 22.42  |
|    | ATOM | 438 | C   | ASP | A | 58 | -7.930  | 49.875 | 60.266 | 1.00 | 27.00  |
|    | ATOM | 439 | O   | ASP | A | 58 | -7.376  | 50.808 | 59.668 | 1.00 | 24.72  |
|    | ATOM | 440 | CB  | ASP | A | 58 | -6.971  | 50.657 | 62.459 | 1.00 | 24.48  |
|    | ATOM | 441 | CG  | ASP | A | 58 | -7.104  | 50.494 | 63.928 | 1.00 | 36.08  |
|    | ATOM | 442 | OD1 | ASP | A | 58 | -8.187  | 50.358 | 64.474 | 1.00 | 38.70  |



|    |      |     |     |     |   |    |         |        |        |      |        |
|----|------|-----|-----|-----|---|----|---------|--------|--------|------|--------|
|    | ATOM | 443 | OD2 | ASP | A | 58 | -5.944  | 50.459 | 64.535 | 1.00 | 37.78  |
|    | ATOM | 444 | N   | LEU | A | 59 | -8.530  | 48.936 | 59.611 | 1.00 | 26.57  |
|    | ATOM | 445 | CA  | LEU | A | 59 | -8.545  | 49.049 | 58.177 | 1.00 | 26.97  |
| 5  | ATOM | 446 | C   | LEU | A | 59 | -9.946  | 49.473 | 57.707 | 1.00 | 30.09  |
|    | ATOM | 447 | O   | LEU | A | 59 | -10.971 | 49.074 | 58.245 | 1.00 | 28.07  |
|    | ATOM | 448 | CB  | LEU | A | 59 | -8.132  | 47.698 | 57.479 | 1.00 | 26.65  |
|    | ATOM | 449 | CG  | LEU | A | 59 | -6.639  | 47.356 | 57.443 | 1.00 | 24.34  |
|    | ATOM | 450 | CD1 | LEU | A | 59 | -6.445  | 46.049 | 56.687 | 1.00 | 25.03  |
| 10 | ATOM | 451 | CD2 | LEU | A | 59 | -5.864  | 48.443 | 56.722 | 1.00 | 21.60  |
|    | ATOM | 452 | N   | THR | A | 60 | -9.982  | 50.278 | 56.673 | 1.00 | 29.73  |
|    | ATOM | 453 | CA  | THR | A | 60 | -11.244 | 50.685 | 56.091 | 1.00 | 30.53  |
|    | ATOM | 454 | C   | THR | A | 60 | -11.433 | 49.876 | 54.791 | 1.00 | 34.07  |
|    | ATOM | 455 | O   | THR | A | 60 | -10.634 | 49.978 | 53.813 | 1.00 | 29.18  |
|    | ATOM | 456 | CB  | THR | A | 60 | -11.282 | 52.198 | 55.881 | 1.00 | 38.77  |
| 15 | ATOM | 457 | OG1 | THR | A | 60 | -11.898 | 52.759 | 57.020 | 1.00 | 55.62  |
|    | ATOM | 458 | CG2 | THR | A | 60 | -12.086 | 52.528 | 54.635 | 1.00 | 42.40  |
|    | ATOM | 459 | N   | ILE | A | 61 | -12.465 | 49.042 | 54.808 | 1.00 | 30.99  |
|    | ATOM | 460 | CA  | ILE | A | 61 | -12.758 | 48.181 | 53.667 | 1.00 | 33.20  |
| 20 | ATOM | 461 | C   | ILE | A | 61 | -13.821 | 48.708 | 52.741 | 1.00 | 38.63  |
|    | ATOM | 462 | O   | ILE | A | 61 | -14.987 | 48.694 | 53.102 | 1.00 | 34.56  |
|    | ATOM | 463 | CB  | ILE | A | 61 | -13.230 | 46.809 | 54.087 | 1.00 | 37.17  |
|    | ATOM | 464 | CG1 | ILE | A | 61 | -12.407 | 46.229 | 55.252 | 1.00 | 37.33  |
|    | ATOM | 465 | CG2 | ILE | A | 61 | -13.229 | 45.905 | 52.850 | 1.00 | 39.90  |
| 25 | ATOM | 466 | CD1 | ILE | A | 61 | -10.929 | 46.003 | 54.937 | 1.00 | 41.79  |
|    | ATOM | 467 | N   | GLU | A | 62 | -13.407 | 49.117 | 51.548 | 1.00 | 42.13  |
|    | ATOM | 468 | CA  | GLU | A | 62 | -14.330 | 49.624 | 50.543 | 1.00 | 45.12  |
|    | ATOM | 469 | C   | GLU | A | 62 | -15.208 | 48.498 | 49.976 | 1.00 | 48.64  |
|    | ATOM | 470 | O   | GLU | A | 62 | -16.442 | 48.537 | 49.984 | 1.00 | 49.46  |
| 30 | ATOM | 471 | CB  | GLU | A | 62 | -13.550 | 50.305 | 49.397 | 1.00 | 47.88  |
|    | ATOM | 472 | CG  | GLU | A | 62 | -14.390 | 51.345 | 48.620 | 1.00 | 73.90  |
|    | ATOM | 473 | CD  | GLU | A | 62 | -15.062 | 50.839 | 47.363 | 1.00 | 100.00 |
|    | ATOM | 474 | OE1 | GLU | A | 62 | -16.062 | 50.129 | 47.371 | 1.00 | 100.00 |
|    | ATOM | 475 | OE2 | GLU | A | 62 | -14.492 | 51.296 | 46.267 | 1.00 | 100.00 |
| 35 | ATOM | 476 | N   | LYS | A | 63 | -14.551 | 47.459 | 49.483 | 1.00 | 40.80  |
|    | ATOM | 477 | CA  | LYS | A | 63 | -15.283 | 46.342 | 48.931 | 1.00 | 36.23  |
|    | ATOM | 478 | C   | LYS | A | 63 | -14.377 | 45.153 | 48.678 | 1.00 | 34.27  |
|    | ATOM | 479 | O   | LYS | A | 63 | -13.167 | 45.306 | 48.512 | 1.00 | 29.28  |
|    | ATOM | 480 | CB  | LYS | A | 63 | -15.891 | 46.760 | 47.601 | 1.00 | 32.16  |
| 40 | ATOM | 481 | CG  | LYS | A | 63 | -14.816 | 47.067 | 46.573 | 1.00 | 22.38  |
|    | ATOM | 482 | CD  | LYS | A | 63 | -15.373 | 47.148 | 45.162 | 1.00 | 32.02  |
|    | ATOM | 483 | CE  | LYS | A | 63 | -14.778 | 48.257 | 44.308 | 1.00 | 33.99  |
|    | ATOM | 484 | NZ  | LYS | A | 63 | -13.723 | 47.814 | 43.365 | 1.00 | 52.00  |
|    | ATOM | 485 | N   | VAL | A | 64 | -15.001 | 43.985 | 48.614 | 1.00 | 36.16  |
| 45 | ATOM | 486 | CA  | VAL | A | 64 | -14.292 | 42.751 | 48.306 | 1.00 | 39.33  |
|    | ATOM | 487 | C   | VAL | A | 64 | -14.792 | 42.157 | 46.993 | 1.00 | 43.15  |
|    | ATOM | 488 | O   | VAL | A | 64 | -15.971 | 41.822 | 46.859 | 1.00 | 38.90  |
|    | ATOM | 489 | CB  | VAL | A | 64 | -14.401 | 41.692 | 49.370 | 1.00 | 42.66  |
|    | ATOM | 490 | CG1 | VAL | A | 64 | -13.465 | 40.566 | 48.928 | 1.00 | 42.11  |
| 50 | ATOM | 491 | CG2 | VAL | A | 64 | -14.028 | 42.276 | 50.730 | 1.00 | 40.96  |
|    | ATOM | 492 | N   | VAL | A | 65 | -13.892 | 42.023 | 46.036 | 1.00 | 40.44  |
|    | ATOM | 493 | CA  | VAL | A | 65 | -14.287 | 41.505 | 44.739 | 1.00 | 37.94  |
|    | ATOM | 494 | C   | VAL | A | 65 | -13.708 | 40.162 | 44.350 | 1.00 | 35.48  |
|    | ATOM | 495 | O   | VAL | A | 65 | -12.511 | 39.915 | 44.474 | 1.00 | 31.12  |
| 55 | ATOM | 496 | CB  | VAL | A | 65 | -14.047 | 42.540 | 43.647 | 1.00 | 39.44  |
|    | ATOM | 497 | CG1 | VAL | A | 65 | -14.238 | 41.899 | 42.287 | 1.00 | 38.78  |
|    | ATOM | 498 | CG2 | VAL | A | 65 | -15.024 | 43.692 | 43.844 | 1.00 | 38.69  |
|    | ATOM | 499 | N   | ILE | A | 66 | -14.599 | 39.316 | 43.847 | 1.00 | 32.12  |
|    | ATOM | 500 | CA  | ILE | A | 66 | -14.223 | 38.010 | 43.372 | 1.00 | 31.54  |
| 60 | ATOM | 501 | C   | ILE | A | 66 | -14.825 | 37.784 | 41.993 | 1.00 | 37.42  |
|    | ATOM | 502 | O   | ILE | A | 66 | -16.033 | 37.896 | 41.794 | 1.00 | 34.45  |
|    | ATOM | 503 | CB  | ILE | A | 66 | -14.602 | 36.884 | 44.313 | 1.00 | 32.82  |
|    | ATOM | 504 | CG1 | ILE | A | 66 | -13.945 | 37.071 | 45.664 | 1.00 | 30.69  |
|    | ATOM | 505 | CG2 | ILE | A | 66 | -14.117 | 35.581 | 43.703 | 1.00 | 32.94  |
|    | ATOM | 506 | CD1 | ILE | A | 66 | -14.478 | 36.125 | 46.731 | 1.00 | 25.31  |



|    |      |     |     |     |   |    |         |        |        |      |        |
|----|------|-----|-----|-----|---|----|---------|--------|--------|------|--------|
|    | ATOM | 507 | N   | ASN | A | 67 | -13.968 | 37.498 | 41.027 | 1.00 | 38.89  |
|    | ATOM | 508 | CA  | ASN | A | 67 | -14.426 | 37.278 | 39.668 | 1.00 | 39.33  |
|    | ATOM | 509 | C   | ASN | A | 67 | -15.373 | 38.366 | 39.223 | 1.00 | 42.51  |
| 5  | ATOM | 510 | O   | ASN | A | 67 | -16.525 | 38.092 | 38.906 | 1.00 | 39.37  |
|    | ATOM | 511 | CB  | ASN | A | 67 | -15.095 | 35.904 | 39.501 | 1.00 | 35.20  |
|    | ATOM | 512 | CG  | ASN | A | 67 | -14.141 | 34.765 | 39.862 | 1.00 | 61.24  |
|    | ATOM | 513 | OD1 | ASN | A | 67 | -12.900 | 34.842 | 39.669 | 1.00 | 47.44  |
|    | ATOM | 514 | ND2 | ASN | A | 67 | -14.717 | 33.706 | 40.421 | 1.00 | 42.22  |
| 10 | ATOM | 515 | N   | GLY | A | 68 | -14.848 | 39.590 | 39.237 | 1.00 | 39.48  |
|    | ATOM | 516 | CA  | GLY | A | 68 | -15.527 | 40.809 | 38.826 | 1.00 | 37.68  |
|    | ATOM | 517 | C   | GLY | A | 68 | -16.763 | 41.167 | 39.612 | 1.00 | 39.81  |
|    | ATOM | 518 | O   | GLY | A | 68 | -17.380 | 42.197 | 39.398 | 1.00 | 43.86  |
|    | ATOM | 519 | N   | GLN | A | 69 | -17.173 | 40.333 | 40.513 | 1.00 | 33.09  |
| 15 | ATOM | 520 | CA  | GLN | A | 69 | -18.351 | 40.732 | 41.230 | 1.00 | 34.40  |
|    | ATOM | 521 | C   | GLN | A | 69 | -17.958 | 41.090 | 42.626 | 1.00 | 47.27  |
|    | ATOM | 522 | O   | GLN | A | 69 | -16.841 | 40.790 | 43.059 | 1.00 | 49.22  |
|    | ATOM | 523 | CB  | GLN | A | 69 | -19.416 | 39.624 | 41.285 | 1.00 | 36.28  |
|    | ATOM | 524 | CG  | GLN | A | 69 | -19.908 | 39.174 | 39.893 | 1.00 | 42.32  |
| 20 | ATOM | 525 | CD  | GLN | A | 69 | -20.467 | 40.321 | 39.111 | 1.00 | 54.27  |
|    | ATOM | 526 | OE1 | GLN | A | 69 | -19.968 | 40.635 | 38.025 | 1.00 | 50.67  |
|    | ATOM | 527 | NE2 | GLN | A | 69 | -21.462 | 40.989 | 39.696 | 1.00 | 59.09  |
|    | ATOM | 528 | N   | GLU | A | 70 | -18.898 | 41.715 | 43.318 | 1.00 | 45.54  |
|    | ATOM | 529 | CA  | GLU | A | 70 | -18.697 | 42.105 | 44.682 | 1.00 | 43.70  |
| 25 | ATOM | 530 | C   | GLU | A | 70 | -19.236 | 40.986 | 45.548 | 1.00 | 50.02  |
|    | ATOM | 531 | O   | GLU | A | 70 | -20.200 | 40.332 | 45.162 | 1.00 | 55.78  |
|    | ATOM | 532 | CB  | GLU | A | 70 | -19.351 | 43.459 | 44.985 | 1.00 | 43.37  |
|    | ATOM | 533 | CG  | GLU | A | 70 | -18.528 | 44.659 | 44.476 | 1.00 | 45.21  |
|    | ATOM | 534 | CD  | GLU | A | 70 | -19.093 | 45.975 | 44.964 | 1.00 | 80.18  |
| 30 | ATOM | 535 | OE1 | GLU | A | 70 | -19.937 | 46.064 | 45.861 | 1.00 | 51.66  |
|    | ATOM | 536 | OE2 | GLU | A | 70 | -18.594 | 47.005 | 44.319 | 1.00 | 79.05  |
|    | ATOM | 537 | N   | VAL | A | 71 | -18.611 | 40.735 | 46.695 | 1.00 | 37.89  |
|    | ATOM | 538 | CA  | VAL | A | 71 | -19.067 | 39.666 | 47.551 | 1.00 | 33.11  |
|    | ATOM | 539 | C   | VAL | A | 71 | -19.420 | 40.129 | 48.963 | 1.00 | 35.14  |
| 35 | ATOM | 540 | O   | VAL | A | 71 | -19.165 | 41.257 | 49.380 | 1.00 | 36.32  |
|    | ATOM | 541 | CB  | VAL | A | 71 | -18.147 | 38.422 | 47.497 | 1.00 | 33.37  |
|    | ATOM | 542 | CG1 | VAL | A | 71 | -17.772 | 38.119 | 46.050 | 1.00 | 31.13  |
|    | ATOM | 543 | CG2 | VAL | A | 71 | -16.866 | 38.594 | 48.326 | 1.00 | 31.47  |
|    | ATOM | 544 | N   | LYS | A | 72 | -20.016 | 39.247 | 49.696 | 1.00 | 31.08  |
| 40 | ATOM | 545 | CA  | LYS | A | 72 | -20.385 | 39.549 | 51.037 | 1.00 | 34.55  |
|    | ATOM | 546 | C   | LYS | A | 72 | -19.155 | 39.360 | 51.922 | 1.00 | 46.45  |
|    | ATOM | 547 | O   | LYS | A | 72 | -18.344 | 38.455 | 51.678 | 1.00 | 44.93  |
|    | ATOM | 548 | CB  | LYS | A | 72 | -21.484 | 38.586 | 51.447 | 1.00 | 37.84  |
|    | ATOM | 549 | CG  | LYS | A | 72 | -22.553 | 39.153 | 52.362 | 1.00 | 60.35  |
| 45 | ATOM | 550 | CD  | LYS | A | 72 | -22.630 | 38.370 | 53.660 | 1.00 | 78.18  |
|    | ATOM | 551 | CE  | LYS | A | 72 | -21.389 | 38.589 | 54.500 | 1.00 | 92.99  |
|    | ATOM | 552 | NZ  | LYS | A | 72 | -20.860 | 39.935 | 54.295 | 1.00 | 100.00 |
|    | ATOM | 553 | N   | TYR | A | 73 | -19.051 | 40.242 | 52.930 | 1.00 | 45.41  |
|    | ATOM | 554 | CA  | TYR | A | 73 | -18.006 | 40.276 | 53.941 | 1.00 | 45.13  |
| 50 | ATOM | 555 | C   | TYR | A | 73 | -18.474 | 41.017 | 55.167 | 1.00 | 47.06  |
|    | ATOM | 556 | O   | TYR | A | 73 | -19.231 | 41.979 | 55.089 | 1.00 | 45.05  |
|    | ATOM | 557 | CB  | TYR | A | 73 | -16.720 | 40.932 | 53.488 | 1.00 | 44.74  |
|    | ATOM | 558 | CG  | TYR | A | 73 | -16.753 | 42.438 | 53.504 | 1.00 | 47.77  |
|    | ATOM | 559 | CD1 | TYR | A | 73 | -16.507 | 43.169 | 54.674 | 1.00 | 50.00  |
| 55 | ATOM | 560 | CD2 | TYR | A | 73 | -17.005 | 43.133 | 52.306 | 1.00 | 49.34  |
|    | ATOM | 561 | CE1 | TYR | A | 73 | -16.519 | 44.565 | 54.662 | 1.00 | 52.06  |
|    | ATOM | 562 | CE2 | TYR | A | 73 | -16.967 | 44.529 | 52.284 | 1.00 | 50.56  |
|    | ATOM | 563 | CZ  | TYR | A | 73 | -16.684 | 45.235 | 53.452 | 1.00 | 60.67  |
|    | ATOM | 564 | OH  | TYR | A | 73 | -16.859 | 46.597 | 53.418 | 1.00 | 66.04  |
| 60 | ATOM | 565 | N   | ALA | A | 74 | -17.993 | 40.557 | 56.289 | 1.00 | 40.33  |
|    | ATOM | 566 | CA  | ALA | A | 74 | -18.323 | 41.138 | 57.545 | 1.00 | 39.85  |
|    | ATOM | 567 | C   | ALA | A | 74 | -17.068 | 41.281 | 58.412 | 1.00 | 47.89  |
|    | ATOM | 568 | O   | ALA | A | 74 | -16.147 | 40.464 | 58.346 | 1.00 | 46.81  |
|    | ATOM | 569 | CB  | ALA | A | 74 | -19.346 | 40.262 | 58.237 | 1.00 | 39.87  |
|    | ATOM | 570 | N   | LEU | A | 75 | -17.055 | 42.339 | 59.227 | 1.00 | 42.79  |



|    |      |     |     |     |   |    |         |        |        |      |        |
|----|------|-----|-----|-----|---|----|---------|--------|--------|------|--------|
|    | ATOM | 571 | CA  | LEU | A | 75 | -15.980 | 42.650 | 60.148 | 1.00 | 38.94  |
|    | ATOM | 572 | C   | LEU | A | 75 | -16.416 | 42.342 | 61.561 | 1.00 | 44.65  |
|    | ATOM | 573 | O   | LEU | A | 75 | -17.388 | 42.895 | 62.068 | 1.00 | 48.50  |
| 5  | ATOM | 574 | CB  | LEU | A | 75 | -15.667 | 44.141 | 60.115 | 1.00 | 37.30  |
|    | ATOM | 575 | CG  | LEU | A | 75 | -14.899 | 44.572 | 58.899 | 1.00 | 44.06  |
|    | ATOM | 576 | CD1 | LEU | A | 75 | -14.476 | 46.031 | 59.085 | 1.00 | 47.51  |
|    | ATOM | 577 | CD2 | LEU | A | 75 | -13.691 | 43.666 | 58.677 | 1.00 | 46.54  |
|    | ATOM | 578 | N   | GLY | A | 76 | -15.718 | 41.474 | 62.242 | 1.00 | 39.16  |
| 10 | ATOM | 579 | CA  | GLY | A | 76 | -16.145 | 41.228 | 63.597 | 1.00 | 36.77  |
|    | ATOM | 580 | C   | GLY | A | 76 | -15.652 | 42.360 | 64.461 | 1.00 | 31.43  |
|    | ATOM | 581 | O   | GLY | A | 76 | -14.997 | 43.290 | 63.969 | 1.00 | 26.07  |
|    | ATOM | 582 | N   | GLU | A | 77 | -15.973 | 42.281 | 65.736 | 1.00 | 32.78  |
|    | ATOM | 583 | CA  | GLU | A | 77 | -15.539 | 43.318 | 66.645 | 1.00 | 34.78  |
|    | ATOM | 584 | C   | GLU | A | 77 | -14.050 | 43.214 | 66.886 | 1.00 | 38.63  |
| 15 | ATOM | 585 | O   | GLU | A | 77 | -13.431 | 42.176 | 66.641 | 1.00 | 34.85  |
|    | ATOM | 586 | CB  | GLU | A | 77 | -16.337 | 43.338 | 67.966 | 1.00 | 37.18  |
|    | ATOM | 587 | CG  | GLU | A | 77 | -16.506 | 41.956 | 68.643 | 1.00 | 56.65  |
|    | ATOM | 588 | CD  | GLU | A | 77 | -16.316 | 41.990 | 70.151 | 1.00 | 100.00 |
| 20 | ATOM | 589 | OE1 | GLU | A | 77 | -16.789 | 42.859 | 70.877 | 1.00 | 100.00 |
|    | ATOM | 590 | OE2 | GLU | A | 77 | -15.603 | 40.975 | 70.597 | 1.00 | 100.00 |
|    | ATOM | 591 | N   | ARG | A | 78 | -13.483 | 44.312 | 67.343 | 1.00 | 37.73  |
|    | ATOM | 592 | CA  | ARG | A | 78 | -12.068 | 44.336 | 67.624 | 1.00 | 37.11  |
|    | ATOM | 593 | C   | ARG | A | 78 | -11.709 | 43.545 | 68.889 | 1.00 | 39.61  |
| 25 | ATOM | 594 | O   | ARG | A | 78 | -12.422 | 43.549 | 69.906 | 1.00 | 36.40  |
|    | ATOM | 595 | CB  | ARG | A | 78 | -11.522 | 45.744 | 67.693 | 1.00 | 33.62  |
|    | ATOM | 596 | CG  | ARG | A | 78 | -9.991  | 45.807 | 67.699 | 1.00 | 34.93  |
|    | ATOM | 597 | CD  | ARG | A | 78 | -9.516  | 47.207 | 68.040 | 1.00 | 32.03  |
|    | ATOM | 598 | NE  | ARG | A | 78 | -8.083  | 47.397 | 68.058 | 1.00 | 33.71  |
| 30 | ATOM | 599 | CZ  | ARG | A | 78 | -7.459  | 48.239 | 67.241 | 1.00 | 53.03  |
|    | ATOM | 600 | NH1 | ARG | A | 78 | -8.114  | 48.941 | 66.314 | 1.00 | 39.56  |
|    | ATOM | 601 | NH2 | ARG | A | 78 | -6.139  | 48.361 | 67.337 | 1.00 | 53.05  |
|    | ATOM | 602 | N   | GLN | A | 79 | -10.576 | 42.842 | 68.795 | 1.00 | 33.34  |
|    | ATOM | 603 | CA  | GLN | A | 79 | -10.044 | 42.052 | 69.881 | 1.00 | 32.25  |
| 35 | ATOM | 604 | C   | GLN | A | 79 | -8.708  | 42.662 | 70.221 | 1.00 | 36.49  |
|    | ATOM | 605 | O   | GLN | A | 79 | -7.651  | 42.164 | 69.834 | 1.00 | 37.41  |
|    | ATOM | 606 | CB  | GLN | A | 79 | -9.906  | 40.580 | 69.472 | 1.00 | 31.80  |
|    | ATOM | 607 | CG  | GLN | A | 79 | -11.263 | 39.972 | 69.092 | 1.00 | 31.70  |
|    | ATOM | 608 | CD  | GLN | A | 79 | -11.143 | 38.511 | 68.713 | 1.00 | 62.24  |
| 40 | ATOM | 609 | OE1 | GLN | A | 79 | -10.234 | 37.819 | 69.182 | 1.00 | 64.13  |
|    | ATOM | 610 | NE2 | GLN | A | 79 | -12.046 | 38.033 | 67.862 | 1.00 | 56.77  |
|    | ATOM | 611 | N   | SER | A | 80 | -8.787  | 43.794 | 70.893 | 1.00 | 30.40  |
|    | ATOM | 612 | CA  | SER | A | 80 | -7.617  | 44.551 | 71.284 | 1.00 | 27.48  |
|    | ATOM | 613 | C   | SER | A | 80 | -6.535  | 44.592 | 70.257 | 1.00 | 29.91  |
| 45 | ATOM | 614 | O   | SER | A | 80 | -6.758  | 45.054 | 69.140 | 1.00 | 28.75  |
|    | ATOM | 615 | CB  | SER | A | 80 | -7.066  | 44.252 | 72.655 | 1.00 | 27.52  |
|    | ATOM | 616 | OG  | SER | A | 80 | -7.173  | 42.874 | 72.863 | 1.00 | 44.76  |
|    | ATOM | 617 | N   | TYR | A | 81 | -5.350  | 44.133 | 70.671 | 1.00 | 27.38  |
|    | ATOM | 618 | CA  | TYR | A | 81 | -4.162  | 44.180 | 69.820 | 1.00 | 25.29  |
| 50 | ATOM | 619 | C   | TYR | A | 81 | -4.196  | 43.286 | 68.604 | 1.00 | 23.60  |
|    | ATOM | 620 | O   | TYR | A | 81 | -3.389  | 43.435 | 67.710 | 1.00 | 26.12  |
|    | ATOM | 621 | CB  | TYR | A | 81 | -2.861  | 43.992 | 70.632 | 1.00 | 23.78  |
|    | ATOM | 622 | CG  | TYR | A | 81 | -2.849  | 42.621 | 71.190 | 1.00 | 21.01  |
|    | ATOM | 623 | CD1 | TYR | A | 81 | -3.374  | 42.361 | 72.450 | 1.00 | 20.45  |
| 55 | ATOM | 624 | CD2 | TYR | A | 81 | -2.387  | 41.569 | 70.406 | 1.00 | 23.13  |
|    | ATOM | 625 | CE1 | TYR | A | 81 | -3.402  | 41.064 | 72.948 | 1.00 | 18.45  |
|    | ATOM | 626 | CE2 | TYR | A | 81 | -2.426  | 40.263 | 70.885 | 1.00 | 24.91  |
|    | ATOM | 627 | CZ  | TYR | A | 81 | -2.929  | 40.017 | 72.162 | 1.00 | 26.97  |
|    | ATOM | 628 | OH  | TYR | A | 81 | -2.960  | 38.731 | 72.652 | 1.00 | 35.08  |
| 60 | ATOM | 629 | N   | LYS | A | 82 | -5.125  | 42.370 | 68.568 | 1.00 | 19.77  |
|    | ATOM | 630 | CA  | LYS | A | 82 | -5.225  | 41.448 | 67.433 | 1.00 | 19.65  |
|    | ATOM | 631 | C   | LYS | A | 82 | -5.948  | 42.036 | 66.232 | 1.00 | 26.75  |
|    | ATOM | 632 | O   | LYS | A | 82 | -5.821  | 41.545 | 65.107 | 1.00 | 26.09  |
|    | ATOM | 633 | CB  | LYS | A | 82 | -5.929  | 40.217 | 67.888 | 1.00 | 19.96  |
|    | ATOM | 634 | CG  | LYS | A | 82 | -5.039  | 39.427 | 68.808 | 1.00 | 39.72  |



|    |      |     |     |     |   |    |         |        |        |      |       |
|----|------|-----|-----|-----|---|----|---------|--------|--------|------|-------|
|    | ATOM | 635 | CD  | LYS | A | 82 | -5.610  | 38.058 | 69.103 | 1.00 | 45.35 |
|    | ATOM | 636 | CE  | LYS | A | 82 | -5.868  | 37.809 | 70.577 | 1.00 | 52.66 |
|    | ATOM | 637 | NZ  | LYS | A | 82 | -6.016  | 36.375 | 70.879 | 1.00 | 51.38 |
| 5  | ATOM | 638 | N   | GLY | A | 83 | -6.698  | 43.114 | 66.482 | 1.00 | 25.62 |
|    | ATOM | 639 | CA  | GLY | A | 83 | -7.465  | 43.786 | 65.441 | 1.00 | 24.64 |
|    | ATOM | 640 | C   | GLY | A | 83 | -8.857  | 43.145 | 65.324 | 1.00 | 26.15 |
|    | ATOM | 641 | O   | GLY | A | 83 | -9.348  | 42.515 | 66.255 | 1.00 | 24.12 |
|    | ATOM | 642 | N   | SER | A | 84 | -9.463  | 43.273 | 64.136 | 1.00 | 27.22 |
| 10 | ATOM | 643 | CA  | SER | A | 84 | -10.806 | 42.770 | 63.829 | 1.00 | 27.17 |
|    | ATOM | 644 | C   | SER | A | 84 | -10.815 | 41.744 | 62.720 | 1.00 | 29.72 |
|    | ATOM | 645 | O   | SER | A | 84 | -10.237 | 41.933 | 61.649 | 1.00 | 30.39 |
|    | ATOM | 646 | CB  | SER | A | 84 | -11.708 | 43.929 | 63.377 | 1.00 | 31.94 |
|    | ATOM | 647 | OG  | SER | A | 84 | -11.719 | 44.976 | 64.344 | 1.00 | 42.05 |
|    | ATOM | 648 | N   | PRO | A | 85 | -11.513 | 40.667 | 62.979 | 1.00 | 24.61 |
| 15 | ATOM | 649 | CA  | PRO | A | 85 | -11.640 | 39.590 | 62.017 | 1.00 | 25.06 |
|    | ATOM | 650 | C   | PRO | A | 85 | -12.480 | 40.005 | 60.819 | 1.00 | 33.19 |
|    | ATOM | 651 | O   | PRO | A | 85 | -13.536 | 40.622 | 60.995 | 1.00 | 31.19 |
|    | ATOM | 652 | CB  | PRO | A | 85 | -12.404 | 38.469 | 62.736 | 1.00 | 24.61 |
| 20 | ATOM | 653 | CG  | PRO | A | 85 | -12.959 | 39.049 | 64.014 | 1.00 | 30.62 |
|    | ATOM | 654 | CD  | PRO | A | 85 | -12.314 | 40.423 | 64.199 | 1.00 | 26.23 |
|    | ATOM | 655 | N   | MET | A | 86 | -12.019 | 39.632 | 59.623 | 1.00 | 28.27 |
|    | ATOM | 656 | CA  | MET | A | 86 | -12.754 | 39.924 | 58.411 | 1.00 | 27.27 |
|    | ATOM | 657 | C   | MET | A | 86 | -13.227 | 38.650 | 57.699 | 1.00 | 32.93 |
| 25 | ATOM | 658 | O   | MET | A | 86 | -12.438 | 37.997 | 57.038 | 1.00 | 27.77 |
|    | ATOM | 659 | CB  | MET | A | 86 | -11.930 | 40.743 | 57.451 | 1.00 | 27.52 |
|    | ATOM | 660 | CG  | MET | A | 86 | -12.756 | 41.222 | 56.274 | 1.00 | 30.43 |
|    | ATOM | 661 | SD  | MET | A | 86 | -11.679 | 41.978 | 55.050 | 1.00 | 37.30 |
|    | ATOM | 662 | CE  | MET | A | 86 | -12.815 | 42.248 | 53.681 | 1.00 | 37.61 |
| 30 | ATOM | 663 | N   | GLU | A | 87 | -14.507 | 38.295 | 57.832 | 1.00 | 34.14 |
|    | ATOM | 664 | CA  | GLU | A | 87 | -15.060 | 37.093 | 57.184 | 1.00 | 36.06 |
|    | ATOM | 665 | C   | GLU | A | 87 | -15.538 | 37.367 | 55.766 | 1.00 | 39.45 |
|    | ATOM | 666 | O   | GLU | A | 87 | -16.366 | 38.250 | 55.586 | 1.00 | 41.63 |
|    | ATOM | 667 | CB  | GLU | A | 87 | -16.211 | 36.499 | 58.003 | 1.00 | 37.41 |
| 35 | ATOM | 668 | CG  | GLU | A | 87 | -16.540 | 35.036 | 57.655 | 1.00 | 43.37 |
|    | ATOM | 669 | CD  | GLU | A | 87 | -17.445 | 34.371 | 58.657 | 1.00 | 60.02 |
|    | ATOM | 670 | OE1 | GLU | A | 87 | -18.629 | 34.637 | 58.785 | 1.00 | 83.59 |
|    | ATOM | 671 | OE2 | GLU | A | 87 | -16.827 | 33.467 | 59.375 | 1.00 | 74.01 |
|    | ATOM | 672 | N   | ILE | A | 88 | -15.000 | 36.608 | 54.788 | 1.00 | 34.85 |
| 40 | ATOM | 673 | CA  | ILE | A | 88 | -15.343 | 36.698 | 53.359 | 1.00 | 33.18 |
|    | ATOM | 674 | C   | ILE | A | 88 | -16.170 | 35.489 | 52.896 | 1.00 | 42.28 |
|    | ATOM | 675 | O   | ILE | A | 88 | -15.895 | 34.352 | 53.254 | 1.00 | 43.61 |
|    | ATOM | 676 | CB  | ILE | A | 88 | -14.122 | 36.878 | 52.475 | 1.00 | 33.03 |
|    | ATOM | 677 | CG1 | ILE | A | 88 | -13.251 | 38.003 | 53.020 | 1.00 | 31.03 |
| 45 | ATOM | 678 | CG2 | ILE | A | 88 | -14.525 | 37.171 | 51.035 | 1.00 | 31.15 |
|    | ATOM | 679 | CD1 | ILE | A | 88 | -12.088 | 38.331 | 52.096 | 1.00 | 33.21 |
|    | ATOM | 680 | N   | SER | A | 89 | -17.222 | 35.723 | 52.116 | 1.00 | 41.90 |
|    | ATOM | 681 | CA  | SER | A | 89 | -18.072 | 34.635 | 51.633 | 1.00 | 40.20 |
|    | ATOM | 682 | C   | SER | A | 89 | -17.689 | 34.229 | 50.234 | 1.00 | 43.89 |
| 50 | ATOM | 683 | O   | SER | A | 89 | -17.731 | 35.037 | 49.296 | 1.00 | 40.79 |
|    | ATOM | 684 | CB  | SER | A | 89 | -19.557 | 34.959 | 51.685 | 1.00 | 43.23 |
|    | ATOM | 685 | OG  | SER | A | 89 | -20.042 | 34.675 | 52.986 | 1.00 | 57.92 |
|    | ATOM | 686 | N   | LEU | A | 90 | -17.298 | 32.967 | 50.099 | 1.00 | 41.94 |
|    | ATOM | 687 | CA  | LEU | A | 90 | -16.945 | 32.481 | 48.793 | 1.00 | 41.32 |
| 55 | ATOM | 688 | C   | LEU | A | 90 | -18.258 | 32.175 | 48.106 | 1.00 | 41.86 |
|    | ATOM | 689 | O   | LEU | A | 90 | -19.186 | 31.608 | 48.692 | 1.00 | 41.35 |
|    | ATOM | 690 | CB  | LEU | A | 90 | -16.014 | 31.252 | 48.856 | 1.00 | 41.25 |
|    | ATOM | 691 | CG  | LEU | A | 90 | -14.827 | 31.484 | 49.781 | 1.00 | 43.31 |
|    | ATOM | 692 | CD1 | LEU | A | 90 | -14.050 | 30.182 | 50.020 | 1.00 | 40.39 |
|    | ATOM | 693 | CD2 | LEU | A | 90 | -13.940 | 32.569 | 49.162 | 1.00 | 40.88 |
| 60 | ATOM | 694 | N   | PRO | A | 91 | -18.337 | 32.612 | 46.887 | 1.00 | 40.52 |
|    | ATOM | 695 | CA  | PRO | A | 91 | -19.516 | 32.434 | 46.056 | 1.00 | 43.11 |
|    | ATOM | 696 | C   | PRO | A | 91 | -19.516 | 31.058 | 45.401 | 1.00 | 51.36 |
|    | ATOM | 697 | O   | PRO | A | 91 | -20.363 | 30.753 | 44.576 | 1.00 | 52.06 |
|    | ATOM | 698 | CB  | PRO | A | 91 | -19.359 | 33.470 | 44.942 | 1.00 | 43.83 |



|    |      |     |     |     |   |    |         |        |        |      |        |
|----|------|-----|-----|-----|---|----|---------|--------|--------|------|--------|
|    | ATOM | 699 | CG  | PRO | A | 91 | -17.883 | 33.867 | 44.915 | 1.00 | 48.09  |
|    | ATOM | 700 | CD  | PRO | A | 91 | -17.268 | 33.373 | 46.217 | 1.00 | 41.44  |
|    | ATOM | 701 | N   | ILE | A | 92 | -18.516 | 30.261 | 45.767 | 1.00 | 50.02  |
| 5  | ATOM | 702 | CA  | ILE | A | 92 | -18.325 | 28.924 | 45.259 | 1.00 | 50.50  |
|    | ATOM | 703 | C   | ILE | A | 92 | -17.525 | 28.128 | 46.242 | 1.00 | 47.69  |
|    | ATOM | 704 | O   | ILE | A | 92 | -16.416 | 28.497 | 46.564 | 1.00 | 46.80  |
|    | ATOM | 705 | CB  | ILE | A | 92 | -17.492 | 28.924 | 44.001 | 1.00 | 55.84  |
|    | ATOM | 706 | CG1 | ILE | A | 92 | -18.372 | 29.135 | 42.791 | 1.00 | 58.16  |
| 10 | ATOM | 707 | CG2 | ILE | A | 92 | -16.776 | 27.584 | 43.884 | 1.00 | 59.08  |
|    | ATOM | 708 | CD1 | ILE | A | 92 | -17.568 | 29.038 | 41.493 | 1.00 | 83.51  |
|    | ATOM | 709 | N   | ALA | A | 93 | -18.047 | 27.023 | 46.683 | 1.00 | 40.78  |
|    | ATOM | 710 | CA  | ALA | A | 93 | -17.280 | 26.257 | 47.599 | 1.00 | 38.66  |
|    | ATOM | 711 | C   | ALA | A | 93 | -16.066 | 25.735 | 46.892 | 1.00 | 45.36  |
| 15 | ATOM | 712 | O   | ALA | A | 93 | -16.141 | 25.391 | 45.720 | 1.00 | 47.87  |
|    | ATOM | 713 | CB  | ALA | A | 93 | -18.114 | 25.149 | 48.205 | 1.00 | 38.35  |
|    | ATOM | 714 | N   | LEU | A | 94 | -14.956 | 25.716 | 47.630 | 1.00 | 42.52  |
|    | ATOM | 715 | CA  | LEU | A | 94 | -13.652 | 25.233 | 47.181 | 1.00 | 41.33  |
|    | ATOM | 716 | C   | LEU | A | 94 | -13.330 | 23.900 | 47.814 | 1.00 | 46.96  |
| 20 | ATOM | 717 | O   | LEU | A | 94 | -13.719 | 23.618 | 48.948 | 1.00 | 45.93  |
|    | ATOM | 718 | CB  | LEU | A | 94 | -12.515 | 26.182 | 47.571 | 1.00 | 39.52  |
|    | ATOM | 719 | CG  | LEU | A | 94 | -12.515 | 27.449 | 46.748 | 1.00 | 44.05  |
|    | ATOM | 720 | CD1 | LEU | A | 94 | -11.153 | 28.133 | 46.829 | 1.00 | 44.88  |
|    | ATOM | 721 | CD2 | LEU | A | 94 | -12.843 | 27.115 | 45.305 | 1.00 | 45.42  |
| 25 | ATOM | 722 | N   | SER | A | 95 | -12.604 | 23.083 | 47.074 | 1.00 | 44.42  |
|    | ATOM | 723 | CA  | SER | A | 95 | -12.221 | 21.807 | 47.591 | 1.00 | 43.44  |
|    | ATOM | 724 | C   | SER | A | 95 | -10.728 | 21.776 | 47.719 | 1.00 | 36.96  |
|    | ATOM | 725 | O   | SER | A | 95 | -10.038 | 22.639 | 47.187 | 1.00 | 33.14  |
|    | ATOM | 726 | CB  | SER | A | 95 | -12.739 | 20.704 | 46.696 | 1.00 | 51.13  |
| 30 | ATOM | 727 | OG  | SER | A | 95 | -14.083 | 20.459 | 47.074 | 1.00 | 60.97  |
|    | ATOM | 728 | N   | LYS | A | 96 | -10.240 | 20.779 | 48.407 | 1.00 | 33.03  |
|    | ATOM | 729 | CA  | LYS | A | 96 | -8.818  | 20.694 | 48.557 | 1.00 | 33.15  |
|    | ATOM | 730 | C   | LYS | A | 96 | -8.122  | 21.204 | 47.321 | 1.00 | 37.16  |
|    | ATOM | 731 | O   | LYS | A | 96 | -8.514  | 20.922 | 46.188 | 1.00 | 38.12  |
| 35 | ATOM | 732 | CB  | LYS | A | 96 | -8.348  | 19.290 | 48.861 | 1.00 | 34.42  |
|    | ATOM | 733 | CG  | LYS | A | 96 | -8.583  | 18.910 | 50.298 | 1.00 | 57.96  |
|    | ATOM | 734 | CD  | LYS | A | 96 | -8.422  | 17.423 | 50.553 | 1.00 | 73.54  |
|    | ATOM | 735 | CE  | LYS | A | 96 | -9.475  | 16.882 | 51.512 | 1.00 | 94.46  |
|    | ATOM | 736 | NZ  | LYS | A | 96 | -9.837  | 15.475 | 51.246 | 1.00 | 100.00 |
| 40 | ATOM | 737 | N   | ASN | A | 97 | -7.069  | 21.958 | 47.573 | 1.00 | 29.05  |
|    | ATOM | 738 | CA  | ASN | A | 97 | -6.213  | 22.528 | 46.568 | 1.00 | 25.85  |
|    | ATOM | 739 | C   | ASN | A | 97 | -6.783  | 23.479 | 45.576 | 1.00 | 31.84  |
|    | ATOM | 740 | O   | ASN | A | 97 | -6.064  | 23.909 | 44.682 | 1.00 | 33.02  |
|    | ATOM | 741 | CB  | ASN | A | 97 | -5.166  | 21.572 | 46.006 | 1.00 | 33.23  |
| 45 | ATOM | 742 | CG  | ASN | A | 97 | -4.289  | 21.018 | 47.135 | 1.00 | 55.19  |
|    | ATOM | 743 | OD1 | ASN | A | 97 | -4.009  | 19.823 | 47.186 | 1.00 | 56.15  |
|    | ATOM | 744 | ND2 | ASN | A | 97 | -3.873  | 21.867 | 48.073 | 1.00 | 43.36  |
|    | ATOM | 745 | N   | GLN | A | 98 | -8.053  | 23.835 | 45.730 | 1.00 | 32.99  |
|    | ATOM | 746 | CA  | GLN | A | 98 | -8.611  | 24.798 | 44.792 | 1.00 | 35.56  |
| 50 | ATOM | 747 | C   | GLN | A | 98 | -8.259  | 26.220 | 45.204 | 1.00 | 40.34  |
|    | ATOM | 748 | O   | GLN | A | 98 | -8.208  | 26.541 | 46.381 | 1.00 | 37.21  |
|    | ATOM | 749 | CB  | GLN | A | 98 | -10.111 | 24.610 | 44.555 | 1.00 | 38.17  |
|    | ATOM | 750 | CG  | GLN | A | 98 | -10.446 | 23.220 | 43.974 | 1.00 | 47.37  |
|    | ATOM | 751 | CD  | GLN | A | 98 | -11.869 | 23.144 | 43.480 | 1.00 | 68.06  |
| 55 | ATOM | 752 | OE1 | GLN | A | 98 | -12.676 | 22.343 | 43.981 | 1.00 | 68.25  |
|    | ATOM | 753 | NE2 | GLN | A | 98 | -12.184 | 24.014 | 42.527 | 1.00 | 58.46  |
|    | ATOM | 754 | N   | GLU | A | 99 | -8.007  | 27.049 | 44.206 | 1.00 | 42.57  |
|    | ATOM | 755 | CA  | GLU | A | 99 | -7.630  | 28.442 | 44.380 | 1.00 | 43.65  |
|    | ATOM | 756 | C   | GLU | A | 99 | -8.649  | 29.427 | 43.778 | 1.00 | 47.15  |
|    | ATOM | 757 | O   | GLU | A | 99 | -9.262  | 29.166 | 42.734 | 1.00 | 44.38  |
| 60 | ATOM | 758 | CB  | GLU | A | 99 | -6.229  | 28.688 | 43.745 | 1.00 | 44.65  |
|    | ATOM | 759 | CG  | GLU | A | 99 | -5.210  | 27.549 | 44.026 | 1.00 | 62.98  |
|    | ATOM | 760 | CD  | GLU | A | 99 | -3.804  | 27.766 | 43.496 | 1.00 | 92.15  |
|    | ATOM | 761 | OE1 | GLU | A | 99 | -3.299  | 28.867 | 43.338 | 1.00 | 100.00 |
|    | ATOM | 762 | OE2 | GLU | A | 99 | -3.191  | 26.625 | 43.252 | 1.00 | 78.70  |



|    |      |     |     |     |   |     |         |        |        |      |       |
|----|------|-----|-----|-----|---|-----|---------|--------|--------|------|-------|
|    | ATOM | 763 | N   | ILE | A | 100 | -8.801  | 30.565 | 44.468 | 1.00 | 41.83 |
|    | ATOM | 764 | CA  | ILE | A | 100 | -9.632  | 31.698 | 44.080 | 1.00 | 38.88 |
|    | ATOM | 765 | C   | ILE | A | 100 | -8.784  | 32.895 | 44.373 | 1.00 | 43.54 |
| 5  | ATOM | 766 | O   | ILE | A | 100 | -7.812  | 32.830 | 45.135 | 1.00 | 42.91 |
|    | ATOM | 767 | CB  | ILE | A | 100 | -10.879 | 31.971 | 44.904 | 1.00 | 42.18 |
|    | ATOM | 768 | CG1 | ILE | A | 100 | -10.849 | 31.355 | 46.271 | 1.00 | 47.13 |
|    | ATOM | 769 | CG2 | ILE | A | 100 | -12.225 | 31.875 | 44.204 | 1.00 | 41.40 |
|    | ATOM | 770 | CD1 | ILE | A | 100 | -10.493 | 32.395 | 47.331 | 1.00 | 74.72 |
| 10 | ATOM | 771 | N   | VAL | A | 101 | -9.156  | 34.001 | 43.784 | 1.00 | 39.29 |
|    | ATOM | 772 | CA  | VAL | A | 101 | -8.461  | 35.229 | 44.067 | 1.00 | 37.27 |
|    | ATOM | 773 | C   | VAL | A | 101 | -9.435  | 36.255 | 44.626 | 1.00 | 39.62 |
|    | ATOM | 774 | O   | VAL | A | 101 | -10.516 | 36.464 | 44.098 | 1.00 | 38.28 |
|    | ATOM | 775 | CB  | VAL | A | 101 | -7.425  | 35.723 | 43.080 | 1.00 | 36.91 |
| 15 | ATOM | 776 | CG1 | VAL | A | 101 | -7.497  | 34.980 | 41.770 | 1.00 | 34.64 |
|    | ATOM | 777 | CG2 | VAL | A | 101 | -7.482  | 37.237 | 42.939 | 1.00 | 35.34 |
|    | ATOM | 778 | N   | ILE | A | 102 | -9.078  | 36.828 | 45.749 | 1.00 | 31.68 |
|    | ATOM | 779 | CA  | ILE | A | 102 | -9.924  | 37.777 | 46.403 | 1.00 | 28.22 |
|    | ATOM | 780 | C   | ILE | A | 102 | -9.328  | 39.135 | 46.284 | 1.00 | 31.14 |
| 20 | ATOM | 781 | O   | ILE | A | 102 | -8.173  | 39.344 | 46.618 | 1.00 | 31.20 |
|    | ATOM | 782 | CB  | ILE | A | 102 | -10.086 | 37.348 | 47.841 | 1.00 | 30.22 |
|    | ATOM | 783 | CG1 | ILE | A | 102 | -10.432 | 35.863 | 47.821 | 1.00 | 30.27 |
|    | ATOM | 784 | CG2 | ILE | A | 102 | -11.214 | 38.112 | 48.495 | 1.00 | 30.53 |
|    | ATOM | 785 | CD1 | ILE | A | 102 | -10.807 | 35.275 | 49.187 | 1.00 | 36.83 |
| 25 | ATOM | 786 | N   | GLU | A | 103 | -10.087 | 40.073 | 45.761 | 1.00 | 26.48 |
|    | ATOM | 787 | CA  | GLU | A | 103 | -9.510  | 41.390 | 45.655 | 1.00 | 30.38 |
|    | ATOM | 788 | C   | GLU | A | 103 | -10.196 | 42.340 | 46.596 | 1.00 | 38.06 |
|    | ATOM | 789 | O   | GLU | A | 103 | -11.400 | 42.583 | 46.488 | 1.00 | 39.31 |
|    | ATOM | 790 | CB  | GLU | A | 103 | -9.496  | 41.944 | 44.256 | 1.00 | 31.96 |
| 30 | ATOM | 791 | CG  | GLU | A | 103 | -9.063  | 43.403 | 44.237 | 1.00 | 41.76 |
|    | ATOM | 792 | CD  | GLU | A | 103 | -9.594  | 44.045 | 43.003 | 1.00 | 80.28 |
|    | ATOM | 793 | OE1 | GLU | A | 103 | -10.653 | 44.658 | 42.976 | 1.00 | 97.93 |
|    | ATOM | 794 | OE2 | GLU | A | 103 | -8.842  | 43.798 | 41.957 | 1.00 | 70.69 |
|    | ATOM | 795 | N   | ILE | A | 104 | -9.409  | 42.831 | 47.536 | 1.00 | 33.55 |
| 35 | ATOM | 796 | CA  | ILE | A | 104 | -9.900  | 43.716 | 48.562 | 1.00 | 30.57 |
|    | ATOM | 797 | C   | ILE | A | 104 | -9.417  | 45.121 | 48.376 | 1.00 | 32.37 |
|    | ATOM | 798 | O   | ILE | A | 104 | -8.209  | 45.395 | 48.262 | 1.00 | 28.32 |
|    | ATOM | 799 | CB  | ILE | A | 104 | -9.522  | 43.227 | 49.955 | 1.00 | 33.68 |
|    | ATOM | 800 | CG1 | ILE | A | 104 | -9.880  | 41.763 | 50.117 | 1.00 | 31.76 |
| 40 | ATOM | 801 | CG2 | ILE | A | 104 | -10.221 | 44.054 | 51.024 | 1.00 | 32.15 |
|    | ATOM | 802 | CD1 | ILE | A | 104 | -9.097  | 41.073 | 51.227 | 1.00 | 34.97 |
|    | ATOM | 803 | N   | SER | A | 105 | -10.433 | 45.980 | 48.336 | 1.00 | 35.99 |
|    | ATOM | 804 | CA  | SER | A | 105 | -10.304 | 47.420 | 48.202 | 1.00 | 37.06 |
|    | ATOM | 805 | C   | SER | A | 105 | -10.231 | 47.965 | 49.624 | 1.00 | 32.66 |
| 45 | ATOM | 806 | O   | SER | A | 105 | -11.184 | 47.854 | 50.409 | 1.00 | 27.10 |
|    | ATOM | 807 | CB  | SER | A | 105 | -11.479 | 48.007 | 47.438 | 1.00 | 41.57 |
|    | ATOM | 808 | OG  | SER | A | 105 | -11.142 | 48.056 | 46.066 | 1.00 | 42.85 |
|    | ATOM | 809 | N   | PHE | A | 106 | -9.069  | 48.495 | 49.970 | 1.00 | 26.79 |
|    | ATOM | 810 | CA  | PHE | A | 106 | -8.932  | 48.950 | 51.316 | 1.00 | 24.44 |
| 50 | ATOM | 811 | C   | PHE | A | 106 | -8.247  | 50.298 | 51.442 | 1.00 | 27.41 |
|    | ATOM | 812 | O   | PHE | A | 106 | -7.592  | 50.835 | 50.512 | 1.00 | 23.66 |
|    | ATOM | 813 | CB  | PHE | A | 106 | -8.098  | 47.870 | 52.069 | 1.00 | 25.82 |
|    | ATOM | 814 | CG  | PHE | A | 106 | -6.659  | 47.899 | 51.602 | 1.00 | 26.84 |
|    | ATOM | 815 | CD1 | PHE | A | 106 | -6.279  | 47.176 | 50.473 | 1.00 | 29.09 |
| 55 | ATOM | 816 | CD2 | PHE | A | 106 | -5.690  | 48.683 | 52.244 | 1.00 | 26.96 |
|    | ATOM | 817 | CE1 | PHE | A | 106 | -4.959  | 47.223 | 50.019 | 1.00 | 30.72 |
|    | ATOM | 818 | CE2 | PHE | A | 106 | -4.371  | 48.760 | 51.788 | 1.00 | 27.84 |
|    | ATOM | 819 | CZ  | PHE | A | 106 | -4.003  | 48.008 | 50.670 | 1.00 | 27.74 |
|    | ATOM | 820 | N   | GLU | A | 107 | -8.390  | 50.814 | 52.669 | 1.00 | 27.81 |
| 60 | ATOM | 821 | CA  | GLU | A | 107 | -7.776  | 52.082 | 53.054 | 1.00 | 30.68 |
|    | ATOM | 822 | C   | GLU | A | 107 | -7.255  | 52.010 | 54.493 | 1.00 | 30.66 |
|    | ATOM | 823 | O   | GLU | A | 107 | -7.991  | 51.628 | 55.409 | 1.00 | 32.52 |
|    | ATOM | 824 | CB  | GLU | A | 107 | -8.744  | 53.268 | 52.866 | 1.00 | 33.19 |
|    | ATOM | 825 | CG  | GLU | A | 107 | -8.059  | 54.652 | 52.795 | 1.00 | 50.92 |
|    | ATOM | 826 | CD  | GLU | A | 107 | -9.053  | 55.794 | 52.621 | 1.00 | 75.89 |



|    |      |     |     |     |   |     |        |        |        |      |        |
|----|------|-----|-----|-----|---|-----|--------|--------|--------|------|--------|
|    | ATOM | 827 | OE1 | GLU | A | 107 | -9.430 | 56.225 | 51.535 | 1.00 | 61.91  |
|    | ATOM | 828 | OE2 | GLU | A | 107 | -9.483 | 56.292 | 53.762 | 1.00 | 47.17  |
|    | ATOM | 829 | N   | THR | A | 108 | -5.978 | 52.366 | 54.682 | 1.00 | 26.11  |
| 5  | ATOM | 830 | CA  | THR | A | 108 | -5.341 | 52.325 | 56.009 | 1.00 | 28.04  |
|    | ATOM | 831 | C   | THR | A | 108 | -5.664 | 53.563 | 56.790 | 1.00 | 32.96  |
|    | ATOM | 832 | O   | THR | A | 108 | -5.881 | 54.618 | 56.202 | 1.00 | 30.16  |
|    | ATOM | 833 | CB  | THR | A | 108 | -3.787 | 52.277 | 55.957 | 1.00 | 35.08  |
|    | ATOM | 834 | OG1 | THR | A | 108 | -3.245 | 53.465 | 55.378 | 1.00 | 29.19  |
| 10 | ATOM | 835 | CG2 | THR | A | 108 | -3.254 | 51.032 | 55.245 | 1.00 | 32.38  |
|    | ATOM | 836 | N   | SER | A | 109 | -5.650 | 53.417 | 58.112 | 1.00 | 28.09  |
|    | ATOM | 837 | CA  | SER | A | 109 | -5.890 | 54.508 | 59.057 | 1.00 | 22.39  |
|    | ATOM | 838 | C   | SER | A | 109 | -4.612 | 55.300 | 59.248 | 1.00 | 26.59  |
|    | ATOM | 839 | O   | SER | A | 109 | -3.497 | 54.766 | 59.191 | 1.00 | 23.06  |
| 15 | ATOM | 840 | CB  | SER | A | 109 | -6.316 | 53.896 | 60.386 | 1.00 | 23.90  |
|    | ATOM | 841 | OG  | SER | A | 109 | -6.087 | 54.804 | 61.448 | 1.00 | 27.48  |
|    | ATOM | 842 | N   | PRO | A | 110 | -4.720 | 56.594 | 59.495 | 1.00 | 28.89  |
|    | ATOM | 843 | CA  | PRO | A | 110 | -3.481 | 57.312 | 59.703 | 1.00 | 27.31  |
|    | ATOM | 844 | C   | PRO | A | 110 | -2.840 | 56.838 | 60.993 | 1.00 | 27.91  |
| 20 | ATOM | 845 | O   | PRO | A | 110 | -1.651 | 57.033 | 61.172 | 1.00 | 28.30  |
|    | ATOM | 846 | CB  | PRO | A | 110 | -3.776 | 58.792 | 59.689 | 1.00 | 28.41  |
|    | ATOM | 847 | CG  | PRO | A | 110 | -5.188 | 58.921 | 59.138 | 1.00 | 33.97  |
|    | ATOM | 848 | CD  | PRO | A | 110 | -5.820 | 57.545 | 59.214 | 1.00 | 30.89  |
|    | ATOM | 849 | N   | LYS | A | 111 | -3.640 | 56.170 | 61.848 | 1.00 | 21.21  |
| 25 | ATOM | 850 | CA  | LYS | A | 111 | -3.137 | 55.620 | 63.098 | 1.00 | 21.20  |
|    | ATOM | 851 | C   | LYS | A | 111 | -2.634 | 54.163 | 62.972 | 1.00 | 24.12  |
|    | ATOM | 852 | O   | LYS | A | 111 | -2.502 | 53.476 | 63.990 | 1.00 | 27.31  |
|    | ATOM | 853 | CB  | LYS | A | 111 | -4.188 | 55.688 | 64.202 | 1.00 | 24.13  |
|    | ATOM | 854 | CG  | LYS | A | 111 | -4.435 | 57.079 | 64.786 | 1.00 | 44.09  |
| 30 | ATOM | 855 | CD  | LYS | A | 111 | -5.146 | 58.027 | 63.832 | 1.00 | 80.95  |
|    | ATOM | 856 | CE  | LYS | A | 111 | -6.627 | 57.733 | 63.614 | 1.00 | 100.00 |
|    | ATOM | 857 | NZ  | LYS | A | 111 | -7.193 | 58.483 | 62.473 | 1.00 | 100.00 |
|    | ATOM | 858 | N   | SER | A | 112 | -2.371 | 53.669 | 61.743 | 1.00 | 21.95  |
|    | ATOM | 859 | CA  | SER | A | 112 | -1.891 | 52.278 | 61.499 | 1.00 | 21.09  |
| 35 | ATOM | 860 | C   | SER | A | 112 | -0.709 | 51.968 | 62.438 | 1.00 | 23.23  |
|    | ATOM | 861 | O   | SER | A | 112 | 0.236  | 52.722 | 62.472 | 1.00 | 25.25  |
|    | ATOM | 862 | CB  | SER | A | 112 | -1.467 | 52.084 | 60.034 | 1.00 | 17.80  |
|    | ATOM | 863 | OG  | SER | A | 112 | -0.821 | 50.850 | 59.845 | 1.00 | 19.72  |
|    | ATOM | 864 | N   | SER | A | 113 | -0.752 | 50.884 | 63.203 | 1.00 | 19.64  |
| 40 | ATOM | 865 | CA  | SER | A | 113 | 0.342  | 50.587 | 64.087 | 1.00 | 16.68  |
|    | ATOM | 866 | C   | SER | A | 113 | 1.539  | 50.087 | 63.316 | 1.00 | 22.16  |
|    | ATOM | 867 | O   | SER | A | 113 | 2.653  | 50.005 | 63.822 | 1.00 | 21.53  |
|    | ATOM | 868 | CB  | SER | A | 113 | -0.061 | 49.633 | 65.183 | 1.00 | 20.15  |
|    | ATOM | 869 | OG  | SER | A | 113 | -0.358 | 48.369 | 64.663 | 1.00 | 23.41  |
| 45 | ATOM | 870 | N   | ALA | A | 114 | 1.325  | 49.741 | 62.059 | 1.00 | 21.04  |
|    | ATOM | 871 | CA  | ALA | A | 114 | 2.432  | 49.266 | 61.221 | 1.00 | 19.34  |
|    | ATOM | 872 | C   | ALA | A | 114 | 3.212  | 50.412 | 60.581 | 1.00 | 20.25  |
|    | ATOM | 873 | O   | ALA | A | 114 | 4.287  | 50.210 | 60.004 | 1.00 | 20.84  |
|    | ATOM | 874 | CB  | ALA | A | 114 | 1.876  | 48.455 | 60.061 | 1.00 | 19.26  |
| 50 | ATOM | 875 | N   | LEU | A | 115 | 2.636  | 51.614 | 60.636 | 1.00 | 17.27  |
|    | ATOM | 876 | CA  | LEU | A | 115 | 3.281  | 52.725 | 59.992 | 1.00 | 19.18  |
|    | ATOM | 877 | C   | LEU | A | 115 | 3.619  | 53.896 | 60.870 | 1.00 | 22.95  |
|    | ATOM | 878 | O   | LEU | A | 115 | 3.042  | 54.162 | 61.924 | 1.00 | 22.70  |
|    | ATOM | 879 | CB  | LEU | A | 115 | 2.418  | 53.298 | 58.851 | 1.00 | 18.69  |
| 55 | ATOM | 880 | CG  | LEU | A | 115 | 1.844  | 52.219 | 57.960 | 1.00 | 24.36  |
|    | ATOM | 881 | CD1 | LEU | A | 115 | 0.784  | 52.871 | 57.078 | 1.00 | 26.30  |
|    | ATOM | 882 | CD2 | LEU | A | 115 | 2.954  | 51.654 | 57.070 | 1.00 | 21.90  |
|    | ATOM | 883 | N   | GLN | A | 116 | 4.573  | 54.621 | 60.358 | 1.00 | 19.91  |
|    | ATOM | 884 | CA  | GLN | A | 116 | 4.959  | 55.857 | 60.974 | 1.00 | 19.64  |
| 60 | ATOM | 885 | C   | GLN | A | 116 | 5.071  | 56.896 | 59.851 | 1.00 | 22.36  |
|    | ATOM | 886 | O   | GLN | A | 116 | 5.898  | 56.769 | 58.943 | 1.00 | 21.29  |
|    | ATOM | 887 | CB  | GLN | A | 116 | 6.195  | 55.857 | 61.891 | 1.00 | 21.78  |
|    | ATOM | 888 | CG  | GLN | A | 116 | 6.297  | 57.220 | 62.637 | 1.00 | 28.22  |
|    | ATOM | 889 | CD  | GLN | A | 116 | 7.539  | 57.423 | 63.481 | 1.00 | 33.89  |
|    | ATOM | 890 | OE1 | GLN | A | 116 | 8.458  | 56.585 | 63.489 | 1.00 | 21.37  |



|    |      |     |     |     |   |     |        |        |        |      |        |
|----|------|-----|-----|-----|---|-----|--------|--------|--------|------|--------|
|    | ATOM | 891 | NE2 | GLN | A | 116 | 7.569  | 58.557 | 64.198 | 1.00 | 25.06  |
|    | ATOM | 892 | N   | TRP | A | 117 | 4.207  | 57.898 | 59.926 | 1.00 | 21.50  |
|    | ATOM | 893 | CA  | TRP | A | 117 | 4.163  | 58.982 | 58.973 | 1.00 | 22.21  |
| 5  | ATOM | 894 | C   | TRP | A | 117 | 4.909  | 60.164 | 59.588 | 1.00 | 24.80  |
|    | ATOM | 895 | O   | TRP | A | 117 | 4.500  | 60.677 | 60.633 | 1.00 | 24.36  |
|    | ATOM | 896 | CB  | TRP | A | 117 | 2.706  | 59.380 | 58.730 | 1.00 | 20.63  |
|    | ATOM | 897 | CG  | TRP | A | 117 | 1.887  | 58.374 | 57.979 | 1.00 | 21.43  |
|    | ATOM | 898 | CD1 | TRP | A | 117 | 1.079  | 57.439 | 58.532 | 1.00 | 24.14  |
| 10 | ATOM | 899 | CD2 | TRP | A | 117 | 1.736  | 58.258 | 56.562 | 1.00 | 20.88  |
|    | ATOM | 900 | NE1 | TRP | A | 117 | 0.467  | 56.706 | 57.553 | 1.00 | 22.57  |
|    | ATOM | 901 | CE2 | TRP | A | 117 | 0.832  | 57.196 | 56.331 | 1.00 | 24.10  |
|    | ATOM | 902 | CE3 | TRP | A | 117 | 2.279  | 58.953 | 55.467 | 1.00 | 23.47  |
|    | ATOM | 903 | CZ2 | TRP | A | 117 | 0.450  | 56.806 | 55.038 | 1.00 | 24.69  |
| 15 | ATOM | 904 | CZ3 | TRP | A | 117 | 1.929  | 58.563 | 54.182 | 1.00 | 26.53  |
|    | ATOM | 905 | CH2 | TRP | A | 117 | 1.022  | 57.503 | 53.974 | 1.00 | 27.59  |
|    | ATOM | 906 | N   | LEU | A | 118 | 6.000  | 60.565 | 58.932 | 1.00 | 19.11  |
|    | ATOM | 907 | CA  | LEU | A | 118 | 6.864  | 61.652 | 59.372 | 1.00 | 20.20  |
|    | ATOM | 908 | C   | LEU | A | 118 | 6.594  | 62.936 | 58.603 | 1.00 | 29.18  |
| 20 | ATOM | 909 | O   | LEU | A | 118 | 6.422  | 62.907 | 57.379 | 1.00 | 29.44  |
|    | ATOM | 910 | CB  | LEU | A | 118 | 8.364  | 61.287 | 59.137 | 1.00 | 21.47  |
|    | ATOM | 911 | CG  | LEU | A | 118 | 8.985  | 60.284 | 60.141 | 1.00 | 28.52  |
|    | ATOM | 912 | CD1 | LEU | A | 118 | 8.137  | 59.016 | 60.275 | 1.00 | 30.03  |
|    | ATOM | 913 | CD2 | LEU | A | 118 | 10.410 | 59.939 | 59.716 | 1.00 | 27.52  |
| 25 | ATOM | 914 | N   | THR | A | 119 | 6.573  | 64.076 | 59.305 | 1.00 | 23.98  |
|    | ATOM | 915 | CA  | THR | A | 119 | 6.379  | 65.362 | 58.636 | 1.00 | 19.34  |
|    | ATOM | 916 | C   | THR | A | 119 | 7.776  | 65.731 | 58.183 | 1.00 | 23.45  |
|    | ATOM | 917 | O   | THR | A | 119 | 8.736  | 65.253 | 58.783 | 1.00 | 24.77  |
|    | ATOM | 918 | CB  | THR | A | 119 | 5.910  | 66.402 | 59.682 | 1.00 | 26.76  |
| 30 | ATOM | 919 | OG1 | THR | A | 119 | 6.915  | 66.529 | 60.673 | 1.00 | 27.33  |
|    | ATOM | 920 | CG2 | THR | A | 119 | 4.637  | 65.950 | 60.390 | 1.00 | 28.42  |
|    | ATOM | 921 | N   | PRO | A | 120 | 7.933  | 66.565 | 57.151 | 1.00 | 22.29  |
|    | ATOM | 922 | CA  | PRO | A | 120 | 9.255  | 66.927 | 56.678 | 1.00 | 22.30  |
|    | ATOM | 923 | C   | PRO | A | 120 | 10.178 | 67.419 | 57.800 | 1.00 | 28.55  |
| 35 | ATOM | 924 | O   | PRO | A | 120 | 11.404 | 67.260 | 57.754 | 1.00 | 27.54  |
|    | ATOM | 925 | CB  | PRO | A | 120 | 9.059  | 68.024 | 55.624 | 1.00 | 23.05  |
|    | ATOM | 926 | CG  | PRO | A | 120 | 7.581  | 68.150 | 55.384 | 1.00 | 24.12  |
|    | ATOM | 927 | CD  | PRO | A | 120 | 6.876  | 67.282 | 56.407 | 1.00 | 21.87  |
|    | ATOM | 928 | N   | GLU | A | 121 | 9.583  | 68.022 | 58.822 | 1.00 | 28.60  |
| 40 | ATOM | 929 | CA  | GLU | A | 121 | 10.366 | 68.529 | 59.937 | 1.00 | 31.89  |
|    | ATOM | 930 | C   | GLU | A | 121 | 11.104 | 67.394 | 60.658 | 1.00 | 37.79  |
|    | ATOM | 931 | O   | GLU | A | 121 | 12.205 | 67.554 | 61.198 | 1.00 | 35.72  |
|    | ATOM | 932 | CB  | GLU | A | 121 | 9.442  | 69.247 | 60.938 | 1.00 | 34.43  |
|    | ATOM | 933 | CG  | GLU | A | 121 | 8.757  | 70.526 | 60.397 | 1.00 | 61.71  |
| 45 | ATOM | 934 | CD  | GLU | A | 121 | 7.773  | 70.370 | 59.250 | 1.00 | 95.37  |
|    | ATOM | 935 | OE1 | GLU | A | 121 | 6.808  | 69.624 | 59.252 | 1.00 | 50.70  |
|    | ATOM | 936 | OE2 | GLU | A | 121 | 8.033  | 71.193 | 58.262 | 1.00 | 100.00 |
|    | ATOM | 937 | N   | GLN | A | 122 | 10.456 | 66.228 | 60.673 | 1.00 | 33.10  |
|    | ATOM | 938 | CA  | GLN | A | 122 | 11.011 | 65.066 | 61.339 | 1.00 | 30.63  |
| 50 | ATOM | 939 | C   | GLN | A | 122 | 12.104 | 64.392 | 60.538 | 1.00 | 33.25  |
|    | ATOM | 940 | O   | GLN | A | 122 | 12.637 | 63.388 | 60.962 | 1.00 | 33.00  |
|    | ATOM | 941 | CB  | GLN | A | 122 | 9.905  | 64.039 | 61.637 | 1.00 | 30.70  |
|    | ATOM | 942 | CG  | GLN | A | 122 | 8.966  | 64.462 | 62.774 | 1.00 | 23.20  |
|    | ATOM | 943 | CD  | GLN | A | 122 | 7.703  | 63.620 | 62.818 | 1.00 | 27.73  |
| 55 | ATOM | 944 | OE1 | GLN | A | 122 | 6.781  | 63.798 | 62.016 | 1.00 | 34.90  |
|    | ATOM | 945 | NE2 | GLN | A | 122 | 7.655  | 62.689 | 63.757 | 1.00 | 30.55  |
|    | ATOM | 946 | N   | THR | A | 123 | 12.427 | 64.912 | 59.356 | 1.00 | 29.61  |
|    | ATOM | 947 | CA  | THR | A | 123 | 13.438 | 64.288 | 58.495 | 1.00 | 27.96  |
|    | ATOM | 948 | C   | THR | A | 123 | 14.730 | 65.030 | 58.506 | 1.00 | 31.63  |
| 60 | ATOM | 949 | O   | THR | A | 123 | 14.831 | 66.111 | 59.060 | 1.00 | 34.46  |
|    | ATOM | 950 | CB  | THR | A | 123 | 12.966 | 64.183 | 57.029 | 1.00 | 24.54  |
|    | ATOM | 951 | OG1 | THR | A | 123 | 12.855 | 65.504 | 56.515 | 1.00 | 28.43  |
|    | ATOM | 952 | CG2 | THR | A | 123 | 11.594 | 63.521 | 56.985 | 1.00 | 18.48  |
|    | ATOM | 953 | N   | SER | A | 124 | 15.712 | 64.440 | 57.870 | 1.00 | 24.71  |
|    | ATOM | 954 | CA  | SER | A | 124 | 16.980 | 65.088 | 57.814 | 1.00 | 25.71  |



|    |      |      |     |           |        |        |        |      |       |
|----|------|------|-----|-----------|--------|--------|--------|------|-------|
|    | ATOM | 955  | C   | SER A 124 | 16.886 | 66.308 | 56.900 | 1.00 | 34.45 |
|    | ATOM | 956  | O   | SER A 124 | 17.399 | 67.377 | 57.227 | 1.00 | 34.98 |
|    | ATOM | 957  | CB  | SER A 124 | 18.094 | 64.182 | 57.317 | 1.00 | 25.78 |
| 5  | ATOM | 958  | OG  | SER A 124 | 18.268 | 63.099 | 58.177 | 1.00 | 34.37 |
|    | ATOM | 959  | N   | GLY A 125 | 16.221 | 66.110 | 55.756 | 1.00 | 32.47 |
|    | ATOM | 960  | CA  | GLY A 125 | 16.042 | 67.119 | 54.717 | 1.00 | 33.54 |
|    | ATOM | 961  | C   | GLY A 125 | 15.086 | 68.279 | 55.024 | 1.00 | 38.01 |
|    | ATOM | 962  | O   | GLY A 125 | 15.226 | 69.371 | 54.450 | 1.00 | 35.01 |
| 10 | ATOM | 963  | N   | LYS A 126 | 14.100 | 68.055 | 55.893 | 1.00 | 32.87 |
|    | ATOM | 964  | CA  | LYS A 126 | 13.181 | 69.126 | 56.236 | 1.00 | 30.74 |
|    | ATOM | 965  | C   | LYS A 126 | 12.281 | 69.626 | 55.101 | 1.00 | 34.13 |
|    | ATOM | 966  | O   | LYS A 126 | 11.453 | 70.517 | 55.351 | 1.00 | 33.10 |
|    | ATOM | 967  | CB  | LYS A 126 | 13.940 | 70.303 | 56.823 | 1.00 | 31.29 |
|    | ATOM | 968  | CG  | LYS A 126 | 15.031 | 69.877 | 57.790 | 1.00 | 34.55 |
| 15 | ATOM | 969  | CD  | LYS A 126 | 14.459 | 69.111 | 58.962 | 1.00 | 40.18 |
|    | ATOM | 970  | CE  | LYS A 126 | 15.496 | 68.661 | 59.973 | 1.00 | 41.28 |
|    | ATOM | 971  | NZ  | LYS A 126 | 14.895 | 67.775 | 60.987 | 1.00 | 46.79 |
|    | ATOM | 972  | N   | GLU A 127 | 12.436 | 69.079 | 53.869 | 1.00 | 27.28 |
| 20 | ATOM | 973  | CA  | GLU A 127 | 11.617 | 69.510 | 52.737 | 1.00 | 26.31 |
|    | ATOM | 974  | C   | GLU A 127 | 10.566 | 68.517 | 52.300 | 1.00 | 35.95 |
|    | ATOM | 975  | O   | GLU A 127 | 9.636  | 68.879 | 51.575 | 1.00 | 35.05 |
|    | ATOM | 976  | CB  | GLU A 127 | 12.460 | 69.926 | 51.535 | 1.00 | 27.71 |
|    | ATOM | 977  | CG  | GLU A 127 | 13.434 | 71.052 | 51.871 | 1.00 | 37.61 |
|    | ATOM | 978  | CD  | GLU A 127 | 12.763 | 72.391 | 51.971 | 1.00 | 42.53 |
| 25 | ATOM | 979  | OE1 | GLU A 127 | 11.816 | 72.730 | 51.272 | 1.00 | 63.41 |
|    | ATOM | 980  | OE2 | GLU A 127 | 13.334 | 73.149 | 52.873 | 1.00 | 42.43 |
|    | ATOM | 981  | N   | HIS A 128 | 10.729 | 67.260 | 52.730 | 1.00 | 32.31 |
|    | ATOM | 982  | CA  | HIS A 128 | 9.786  | 66.221 | 52.395 | 1.00 | 29.92 |
| 30 | ATOM | 983  | C   | HIS A 128 | 9.400  | 65.337 | 53.570 | 1.00 | 27.82 |
|    | ATOM | 984  | O   | HIS A 128 | 10.117 | 65.179 | 54.549 | 1.00 | 29.92 |
|    | ATOM | 985  | CB  | HIS A 128 | 10.345 | 65.324 | 51.308 | 1.00 | 29.24 |
|    | ATOM | 986  | CG  | HIS A 128 | 10.843 | 66.080 | 50.152 | 1.00 | 31.61 |
|    | ATOM | 987  | ND1 | HIS A 128 | 9.978  | 66.601 | 49.205 | 1.00 | 33.89 |
| 35 | ATOM | 988  | CD2 | HIS A 128 | 12.113 | 66.358 | 49.795 | 1.00 | 34.18 |
|    | ATOM | 989  | CE1 | HIS A 128 | 10.738 | 67.176 | 48.294 | 1.00 | 33.86 |
|    | ATOM | 990  | NE2 | HIS A 128 | 12.030 | 67.053 | 48.618 | 1.00 | 34.37 |
|    | ATOM | 991  | N   | PRO A 129 | 8.261  | 64.747 | 53.430 | 1.00 | 21.92 |
|    | ATOM | 992  | CA  | PRO A 129 | 7.756  | 63.846 | 54.424 | 1.00 | 21.51 |
| 40 | ATOM | 993  | C   | PRO A 129 | 8.419  | 62.474 | 54.216 | 1.00 | 26.61 |
|    | ATOM | 994  | O   | PRO A 129 | 9.302  | 62.284 | 53.376 | 1.00 | 25.02 |
|    | ATOM | 995  | CB  | PRO A 129 | 6.265  | 63.736 | 54.162 | 1.00 | 21.80 |
|    | ATOM | 996  | CG  | PRO A 129 | 6.098  | 64.059 | 52.690 | 1.00 | 28.71 |
|    | ATOM | 997  | CD  | PRO A 129 | 7.353  | 64.818 | 52.263 | 1.00 | 23.90 |
| 45 | ATOM | 998  | N   | TYR A 130 | 8.016  | 61.498 | 54.998 | 1.00 | 22.26 |
|    | ATOM | 999  | CA  | TYR A 130 | 8.646  | 60.195 | 54.881 | 1.00 | 20.30 |
|    | ATOM | 1000 | C   | TYR A 130 | 7.747  | 59.148 | 55.492 | 1.00 | 23.74 |
|    | ATOM | 1001 | O   | TYR A 130 | 7.022  | 59.381 | 56.442 | 1.00 | 23.54 |
|    | ATOM | 1002 | CB  | TYR A 130 | 9.959  | 60.250 | 55.663 | 1.00 | 20.15 |
| 50 | ATOM | 1003 | CG  | TYR A 130 | 10.909 | 59.072 | 55.574 | 1.00 | 23.26 |
|    | ATOM | 1004 | CD1 | TYR A 130 | 10.623 | 57.805 | 56.104 | 1.00 | 23.27 |
|    | ATOM | 1005 | CD2 | TYR A 130 | 12.148 | 59.271 | 54.966 | 1.00 | 24.16 |
|    | ATOM | 1006 | CE1 | TYR A 130 | 11.555 | 56.765 | 56.013 | 1.00 | 20.09 |
|    | ATOM | 1007 | CE2 | TYR A 130 | 13.100 | 58.255 | 54.888 | 1.00 | 23.94 |
| 55 | ATOM | 1008 | CZ  | TYR A 130 | 12.795 | 57.001 | 55.410 | 1.00 | 19.50 |
|    | ATOM | 1009 | OH  | TYR A 130 | 13.751 | 56.053 | 55.281 | 1.00 | 24.55 |
|    | ATOM | 1010 | N   | LEU A 131 | 7.764  | 57.970 | 54.948 | 1.00 | 21.39 |
|    | ATOM | 1011 | CA  | LEU A 131 | 6.916  | 56.975 | 55.551 | 1.00 | 23.29 |
|    | ATOM | 1012 | C   | LEU A 131 | 7.671  | 55.654 | 55.583 | 1.00 | 26.48 |
| 60 | ATOM | 1013 | O   | LEU A 131 | 8.450  | 55.368 | 54.658 | 1.00 | 22.90 |
|    | ATOM | 1014 | CB  | LEU A 131 | 5.632  | 56.805 | 54.721 | 1.00 | 22.31 |
|    | ATOM | 1015 | CG  | LEU A 131 | 4.960  | 55.462 | 54.943 | 1.00 | 24.82 |
|    | ATOM | 1016 | CD1 | LEU A 131 | 4.060  | 55.574 | 56.168 | 1.00 | 24.09 |
|    | ATOM | 1017 | CD2 | LEU A 131 | 4.166  | 55.056 | 53.690 | 1.00 | 23.63 |
|    | ATOM | 1018 | N   | PHE A 132 | 7.463  | 54.866 | 56.631 | 1.00 | 24.01 |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
|    | ATOM | 1019 | CA  | PHE | A | 132 | 8.101  | 53.539 | 56.711 | 1.00 | 23.69 |
|    | ATOM | 1020 | C   | PHE | A | 132 | 7.231  | 52.575 | 57.474 | 1.00 | 23.59 |
|    | ATOM | 1021 | O   | PHE | A | 132 | 6.529  | 52.952 | 58.394 | 1.00 | 20.95 |
| 5  | ATOM | 1022 | CB  | PHE | A | 132 | 9.545  | 53.507 | 57.253 | 1.00 | 25.79 |
|    | ATOM | 1023 | CG  | PHE | A | 132 | 9.654  | 53.806 | 58.740 | 1.00 | 26.81 |
|    | ATOM | 1024 | CD1 | PHE | A | 132 | 9.338  | 52.852 | 59.713 | 1.00 | 26.02 |
|    | ATOM | 1025 | CD2 | PHE | A | 132 | 10.102 | 55.055 | 59.169 | 1.00 | 24.48 |
|    | ATOM | 1026 | CE1 | PHE | A | 132 | 9.458  | 53.144 | 61.074 | 1.00 | 24.42 |
| 10 | ATOM | 1027 | CE2 | PHE | A | 132 | 10.230 | 55.362 | 60.525 | 1.00 | 23.41 |
|    | ATOM | 1028 | CZ  | PHE | A | 132 | 9.900  | 54.403 | 61.485 | 1.00 | 19.60 |
|    | ATOM | 1029 | N   | SER | A | 133 | 7.246  | 51.322 | 57.103 | 1.00 | 20.10 |
|    | ATOM | 1030 | CA  | SER | A | 133 | 6.434  | 50.355 | 57.804 | 1.00 | 17.87 |
|    | ATOM | 1031 | C   | SER | A | 133 | 7.320  | 49.461 | 58.639 | 1.00 | 18.33 |
| 15 | ATOM | 1032 | O   | SER | A | 133 | 8.539  | 49.439 | 58.517 | 1.00 | 21.07 |
|    | ATOM | 1033 | CB  | SER | A | 133 | 5.739  | 49.451 | 56.811 | 1.00 | 24.24 |
|    | ATOM | 1034 | OG  | SER | A | 133 | 6.735  | 48.694 | 56.128 | 1.00 | 24.12 |
|    | ATOM | 1035 | N   | GLN | A | 134 | 6.659  | 48.710 | 59.463 | 1.00 | 15.44 |
|    | ATOM | 1036 | CA  | GLN | A | 134 | 7.268  | 47.748 | 60.340 | 1.00 | 16.95 |
| 20 | ATOM | 1037 | C   | GLN | A | 134 | 6.181  | 46.760 | 60.729 | 1.00 | 21.06 |
|    | ATOM | 1038 | O   | GLN | A | 134 | 5.401  | 46.994 | 61.632 | 1.00 | 22.06 |
|    | ATOM | 1039 | CB  | GLN | A | 134 | 7.966  | 48.415 | 61.526 | 1.00 | 16.26 |
|    | ATOM | 1040 | CG  | GLN | A | 134 | 8.392  | 47.346 | 62.549 | 1.00 | 24.87 |
|    | ATOM | 1041 | CD  | GLN | A | 134 | 9.424  | 46.414 | 61.955 | 1.00 | 36.09 |
|    | ATOM | 1042 | OE1 | GLN | A | 134 | 10.363 | 46.862 | 61.280 | 1.00 | 25.12 |
| 25 | ATOM | 1043 | NE2 | GLN | A | 134 | 9.242  | 45.111 | 62.187 | 1.00 | 30.48 |
|    | ATOM | 1044 | N   | CYS | A | 135 | 6.076  | 45.647 | 60.013 | 1.00 | 15.84 |
|    | ATOM | 1045 | CA  | CYS | A | 135 | 5.025  | 44.712 | 60.313 | 1.00 | 16.52 |
|    | ATOM | 1046 | C   | CYS | A | 135 | 5.298  | 43.683 | 61.381 | 1.00 | 18.38 |
| 30 | ATOM | 1047 | O   | CYS | A | 135 | 4.354  | 43.170 | 61.995 | 1.00 | 19.10 |
|    | ATOM | 1048 | CB  | CYS | A | 135 | 4.649  | 43.908 | 59.067 | 1.00 | 20.50 |
|    | ATOM | 1049 | SG  | CYS | A | 135 | 4.051  | 44.971 | 57.762 | 1.00 | 25.25 |
|    | ATOM | 1050 | N   | GLN | A | 136 | 6.545  | 43.284 | 61.564 | 1.00 | 16.69 |
|    | ATOM | 1051 | CA  | GLN | A | 136 | 6.756  | 42.242 | 62.572 | 1.00 | 16.53 |
| 35 | ATOM | 1052 | C   | GLN | A | 136 | 6.454  | 42.824 | 63.926 | 1.00 | 20.04 |
|    | ATOM | 1053 | O   | GLN | A | 136 | 6.853  | 43.946 | 64.194 | 1.00 | 21.71 |
|    | ATOM | 1054 | CB  | GLN | A | 136 | 8.204  | 41.703 | 62.520 | 1.00 | 18.54 |
|    | ATOM | 1055 | CG  | GLN | A | 136 | 8.488  | 40.565 | 63.533 | 1.00 | 16.78 |
|    | ATOM | 1056 | CD  | GLN | A | 136 | 9.930  | 40.052 | 63.434 | 1.00 | 27.57 |
| 40 | ATOM | 1057 | OE1 | GLN | A | 136 | 10.835 | 40.746 | 62.930 | 1.00 | 19.61 |
|    | ATOM | 1058 | NE2 | GLN | A | 136 | 10.141 | 38.826 | 63.903 | 1.00 | 25.09 |
|    | ATOM | 1059 | N   | ALA | A | 137 | 5.730  | 42.087 | 64.769 | 1.00 | 16.79 |
|    | ATOM | 1060 | CA  | ALA | A | 137 | 5.243  | 40.724 | 64.514 | 1.00 | 16.58 |
|    | ATOM | 1061 | C   | ALA | A | 137 | 3.931  | 40.636 | 63.807 | 1.00 | 20.75 |
| 45 | ATOM | 1062 | O   | ALA | A | 137 | 3.798  | 39.912 | 62.836 | 1.00 | 19.63 |
|    | ATOM | 1063 | CB  | ALA | A | 137 | 5.087  | 39.918 | 65.813 | 1.00 | 16.76 |
|    | ATOM | 1064 | N   | ILE | A | 138 | 2.951  | 41.338 | 64.321 | 1.00 | 18.31 |
|    | ATOM | 1065 | CA  | ILE | A | 138 | 1.647  | 41.247 | 63.721 | 1.00 | 18.68 |
|    | ATOM | 1066 | C   | ILE | A | 138 | 1.065  | 42.566 | 63.294 | 1.00 | 19.68 |
| 50 | ATOM | 1067 | O   | ILE | A | 138 | -0.053 | 42.896 | 63.633 | 1.00 | 21.65 |
|    | ATOM | 1068 | CB  | ILE | A | 138 | 0.727  | 40.532 | 64.692 | 1.00 | 20.75 |
|    | ATOM | 1069 | CG1 | ILE | A | 138 | 0.761  | 41.275 | 66.024 | 1.00 | 21.55 |
|    | ATOM | 1070 | CG2 | ILE | A | 138 | 1.241  | 39.124 | 64.882 | 1.00 | 17.75 |
|    | ATOM | 1071 | CD1 | ILE | A | 138 | -0.211 | 40.698 | 67.044 | 1.00 | 23.44 |
| 55 | ATOM | 1072 | N   | HIS | A | 139 | 1.789  | 43.309 | 62.525 | 1.00 | 19.15 |
|    | ATOM | 1073 | CA  | HIS | A | 139 | 1.231  | 44.581 | 62.113 | 1.00 | 19.05 |
|    | ATOM | 1074 | C   | HIS | A | 139 | 0.899  | 44.615 | 60.644 | 1.00 | 23.60 |
|    | ATOM | 1075 | O   | HIS | A | 139 | 0.427  | 45.604 | 60.127 | 1.00 | 25.90 |
|    | ATOM | 1076 | CB  | HIS | A | 139 | 2.149  | 45.781 | 62.471 | 1.00 | 19.09 |
|    | ATOM | 1077 | CG  | HIS | A | 139 | 2.429  | 45.870 | 63.961 | 1.00 | 21.83 |
| 60 | ATOM | 1078 | ND1 | HIS | A | 139 | 1.476  | 46.324 | 64.872 | 1.00 | 22.32 |
|    | ATOM | 1079 | CD2 | HIS | A | 139 | 3.547  | 45.567 | 64.661 | 1.00 | 21.82 |
|    | ATOM | 1080 | CE1 | HIS | A | 139 | 2.022  | 46.253 | 66.072 | 1.00 | 21.72 |
|    | ATOM | 1081 | NE2 | HIS | A | 139 | 3.259  | 45.811 | 65.980 | 1.00 | 21.41 |
|    | ATOM | 1082 | N   | CYS | A | 140 | 1.175  | 43.545 | 59.942 | 1.00 | 21.39 |



|    |      |      |     |           |        |        |        |      |       |
|----|------|------|-----|-----------|--------|--------|--------|------|-------|
|    | ATOM | 1083 | CA  | CYS A 140 | 0.854  | 43.573 | 58.525 | 1.00 | 21.71 |
|    | ATOM | 1084 | C   | CYS A 140 | -0.630 | 43.848 | 58.327 | 1.00 | 20.64 |
|    | ATOM | 1085 | O   | CYS A 140 | -1.071 | 44.542 | 57.405 | 1.00 | 21.98 |
| 5  | ATOM | 1086 | CB  | CYS A 140 | 1.237  | 42.260 | 57.823 | 1.00 | 22.30 |
|    | ATOM | 1087 | SG  | CYS A 140 | 1.089  | 42.457 | 56.029 | 1.00 | 27.57 |
|    | ATOM | 1088 | N   | ARG A 141 | -1.384 | 43.259 | 59.232 | 1.00 | 18.28 |
|    | ATOM | 1089 | CA  | ARG A 141 | -2.819 | 43.369 | 59.261 | 1.00 | 20.32 |
|    | ATOM | 1090 | C   | ARG A 141 | -3.265 | 44.823 | 59.352 | 1.00 | 27.93 |
| 10 | ATOM | 1091 | O   | ARG A 141 | -4.438 | 45.135 | 59.078 | 1.00 | 29.72 |
|    | ATOM | 1092 | CB  | ARG A 141 | -3.436 | 42.518 | 60.369 | 1.00 | 16.68 |
|    | ATOM | 1093 | CG  | ARG A 141 | -3.035 | 42.944 | 61.781 | 1.00 | 18.27 |
|    | ATOM | 1094 | CD  | ARG A 141 | -3.571 | 41.985 | 62.866 | 1.00 | 15.44 |
|    | ATOM | 1095 | NE  | ARG A 141 | -2.857 | 40.717 | 62.896 | 1.00 | 20.15 |
|    | ATOM | 1096 | CZ  | ARG A 141 | -2.996 | 39.785 | 63.813 | 1.00 | 20.72 |
| 15 | ATOM | 1097 | NH1 | ARG A 141 | -3.825 | 39.908 | 64.827 | 1.00 | 16.67 |
|    | ATOM | 1098 | NH2 | ARG A 141 | -2.258 | 38.692 | 63.685 | 1.00 | 22.83 |
|    | ATOM | 1099 | N   | ALA A 142 | -2.314 | 45.707 | 59.754 | 1.00 | 18.15 |
|    | ATOM | 1100 | CA  | ALA A 142 | -2.599 | 47.127 | 59.901 | 1.00 | 17.64 |
|    | ATOM | 1101 | C   | ALA A 142 | -2.265 | 47.823 | 58.619 | 1.00 | 22.89 |
| 20 | ATOM | 1102 | O   | ALA A 142 | -2.296 | 49.024 | 58.506 | 1.00 | 22.38 |
|    | ATOM | 1103 | CB  | ALA A 142 | -1.908 | 47.771 | 61.085 | 1.00 | 17.04 |
|    | ATOM | 1104 | N   | ILE A 143 | -1.925 | 47.041 | 57.621 | 1.00 | 24.40 |
|    | ATOM | 1105 | CA  | ILE A 143 | -1.634 | 47.632 | 56.341 | 1.00 | 25.97 |
|    | ATOM | 1106 | C   | ILE A 143 | -2.641 | 47.117 | 55.334 | 1.00 | 33.49 |
| 25 | ATOM | 1107 | O   | ILE A 143 | -3.259 | 47.865 | 54.585 | 1.00 | 36.37 |
|    | ATOM | 1108 | CB  | ILE A 143 | -0.222 | 47.447 | 55.839 | 1.00 | 29.94 |
|    | ATOM | 1109 | CG1 | ILE A 143 | 0.791  | 47.972 | 56.853 | 1.00 | 29.88 |
|    | ATOM | 1110 | CG2 | ILE A 143 | -0.094 | 48.232 | 54.533 | 1.00 | 33.06 |
|    | ATOM | 1111 | CD1 | ILE A 143 | 2.224  | 47.722 | 56.389 | 1.00 | 26.42 |
| 30 | ATOM | 1112 | N   | LEU A 144 | -2.843 | 45.822 | 55.350 | 1.00 | 28.38 |
|    | ATOM | 1113 | CA  | LEU A 144 | -3.815 | 45.204 | 54.438 | 1.00 | 29.40 |
|    | ATOM | 1114 | C   | LEU A 144 | -4.421 | 43.917 | 55.030 | 1.00 | 33.99 |
|    | ATOM | 1115 | O   | LEU A 144 | -3.928 | 43.349 | 56.037 | 1.00 | 30.51 |
|    | ATOM | 1116 | CB  | LEU A 144 | -3.213 | 44.969 | 53.037 | 1.00 | 30.43 |
| 35 | ATOM | 1117 | CG  | LEU A 144 | -1.868 | 44.266 | 53.111 | 1.00 | 33.80 |
|    | ATOM | 1118 | CD1 | LEU A 144 | -2.073 | 42.761 | 53.007 | 1.00 | 35.20 |
|    | ATOM | 1119 | CD2 | LEU A 144 | -0.935 | 44.758 | 52.023 | 1.00 | 38.26 |
|    | ATOM | 1120 | N   | PRO A 145 | -5.507 | 43.446 | 54.432 | 1.00 | 27.43 |
|    | ATOM | 1121 | CA  | PRO A 145 | -6.094 | 42.259 | 54.979 | 1.00 | 25.19 |
| 40 | ATOM | 1122 | C   | PRO A 145 | -5.294 | 41.059 | 54.513 | 1.00 | 23.80 |
|    | ATOM | 1123 | O   | PRO A 145 | -4.832 | 41.009 | 53.376 | 1.00 | 23.96 |
|    | ATOM | 1124 | CB  | PRO A 145 | -7.567 | 42.266 | 54.566 | 1.00 | 27.07 |
|    | ATOM | 1125 | CG  | PRO A 145 | -7.810 | 43.609 | 53.886 | 1.00 | 31.08 |
|    | ATOM | 1126 | CD  | PRO A 145 | -6.445 | 44.131 | 53.505 | 1.00 | 26.31 |
| 45 | ATOM | 1127 | N   | CYS A 146 | -5.080 | 40.145 | 55.448 | 1.00 | 23.01 |
|    | ATOM | 1128 | CA  | CYS A 146 | -4.272 | 38.956 | 55.215 | 1.00 | 24.70 |
|    | ATOM | 1129 | C   | CYS A 146 | -4.329 | 37.973 | 56.367 | 1.00 | 28.20 |
|    | ATOM | 1130 | O   | CYS A 146 | -4.966 | 38.211 | 57.413 | 1.00 | 23.14 |
|    | ATOM | 1131 | CB  | CYS A 146 | -2.793 | 39.335 | 55.036 | 1.00 | 25.42 |
| 50 | ATOM | 1132 | SG  | CYS A 146 | -2.164 | 40.274 | 56.463 | 1.00 | 31.88 |
|    | ATOM | 1133 | N   | GLN A 147 | -3.647 | 36.843 | 56.134 | 1.00 | 22.82 |
|    | ATOM | 1134 | CA  | GLN A 147 | -3.522 | 35.796 | 57.127 | 1.00 | 23.08 |
|    | ATOM | 1135 | C   | GLN A 147 | -2.238 | 36.197 | 57.832 | 1.00 | 28.00 |
|    | ATOM | 1136 | O   | GLN A 147 | -1.131 | 35.841 | 57.415 | 1.00 | 25.08 |
| 55 | ATOM | 1137 | CB  | GLN A 147 | -3.346 | 34.427 | 56.449 | 1.00 | 24.85 |
|    | ATOM | 1138 | CG  | GLN A 147 | -4.671 | 33.762 | 56.084 | 1.00 | 19.17 |
|    | ATOM | 1139 | CD  | GLN A 147 | -4.391 | 32.428 | 55.427 | 1.00 | 25.96 |
|    | ATOM | 1140 | OE1 | GLN A 147 | -3.871 | 32.408 | 54.311 | 1.00 | 20.64 |
|    | ATOM | 1141 | NE2 | GLN A 147 | -4.680 | 31.326 | 56.117 | 1.00 | 20.44 |
| 60 | ATOM | 1142 | N   | ASP A 148 | -2.408 | 37.011 | 58.860 | 1.00 | 23.32 |
|    | ATOM | 1143 | CA  | ASP A 148 | -1.295 | 37.566 | 59.587 | 1.00 | 23.26 |
|    | ATOM | 1144 | C   | ASP A 148 | -0.627 | 36.639 | 60.595 | 1.00 | 23.40 |
|    | ATOM | 1145 | O   | ASP A 148 | -0.574 | 36.941 | 61.790 | 1.00 | 24.25 |
|    | ATOM | 1146 | CB  | ASP A 148 | -1.665 | 38.916 | 60.237 | 1.00 | 24.70 |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
|    | ATOM | 1147 | CG  | ASP | A | 148 | -0.440 | 39.722 | 60.517 | 1.00 | 27.92 |
|    | ATOM | 1148 | OD1 | ASP | A | 148 | 0.678  | 39.389 | 60.113 | 1.00 | 27.89 |
|    | ATOM | 1149 | OD2 | ASP | A | 148 | -0.695 | 40.795 | 61.224 | 1.00 | 19.92 |
| 5  | ATOM | 1150 | N   | THR | A | 149 | -0.099 | 35.537 | 60.060 | 1.00 | 19.68 |
|    | ATOM | 1151 | CA  | THR | A | 149 | 0.607  | 34.501 | 60.793 | 1.00 | 18.44 |
|    | ATOM | 1152 | C   | THR | A | 149 | 1.818  | 34.079 | 59.981 | 1.00 | 23.20 |
|    | ATOM | 1153 | O   | THR | A | 149 | 1.761  | 34.027 | 58.741 | 1.00 | 18.98 |
|    | ATOM | 1154 | CB  | THR | A | 149 | -0.261 | 33.256 | 61.004 | 1.00 | 29.08 |
| 10 | ATOM | 1155 | OG1 | THR | A | 149 | 0.577  | 32.168 | 61.421 | 1.00 | 24.67 |
|    | ATOM | 1156 | CG2 | THR | A | 149 | -0.979 | 32.910 | 59.680 | 1.00 | 23.64 |
|    | ATOM | 1157 | N   | PRO | A | 150 | 2.921  | 33.765 | 60.686 | 1.00 | 21.90 |
|    | ATOM | 1158 | CA  | PRO | A | 150 | 4.159  | 33.323 | 60.016 | 1.00 | 19.21 |
|    | ATOM | 1159 | C   | PRO | A | 150 | 4.018  | 31.886 | 59.479 | 1.00 | 21.32 |
| 15 | ATOM | 1160 | O   | PRO | A | 150 | 4.898  | 31.352 | 58.829 | 1.00 | 18.90 |
|    | ATOM | 1161 | CB  | PRO | A | 150 | 5.260  | 33.356 | 61.103 | 1.00 | 19.24 |
|    | ATOM | 1162 | CG  | PRO | A | 150 | 4.544  | 33.455 | 62.444 | 1.00 | 20.32 |
|    | ATOM | 1163 | CD  | PRO | A | 150 | 3.125  | 33.922 | 62.168 | 1.00 | 20.18 |
|    | ATOM | 1164 | N   | SER | A | 151 | 2.902  | 31.226 | 59.771 | 1.00 | 18.68 |
| 20 | ATOM | 1165 | CA  | SER | A | 151 | 2.737  | 29.862 | 59.276 | 1.00 | 20.66 |
|    | ATOM | 1166 | C   | SER | A | 151 | 2.351  | 29.863 | 57.820 | 1.00 | 22.40 |
|    | ATOM | 1167 | O   | SER | A | 151 | 2.295  | 28.836 | 57.199 | 1.00 | 26.24 |
|    | ATOM | 1168 | CB  | SER | A | 151 | 1.674  | 29.117 | 60.057 | 1.00 | 25.01 |
|    | ATOM | 1169 | OG  | SER | A | 151 | 0.444  | 29.814 | 59.897 | 1.00 | 32.09 |
| 25 | ATOM | 1170 | N   | VAL | A | 152 | 2.086  | 31.017 | 57.282 | 1.00 | 18.17 |
|    | ATOM | 1171 | CA  | VAL | A | 152 | 1.696  | 31.105 | 55.899 | 1.00 | 20.54 |
|    | ATOM | 1172 | C   | VAL | A | 152 | 2.740  | 31.874 | 55.088 | 1.00 | 26.40 |
|    | ATOM | 1173 | O   | VAL | A | 152 | 3.159  | 32.955 | 55.494 | 1.00 | 25.43 |
|    | ATOM | 1174 | CB  | VAL | A | 152 | 0.307  | 31.756 | 55.773 | 1.00 | 22.01 |
| 30 | ATOM | 1175 | CG1 | VAL | A | 152 | 0.000  | 32.092 | 54.316 | 1.00 | 21.07 |
|    | ATOM | 1176 | CG2 | VAL | A | 152 | -0.742 | 30.818 | 56.325 | 1.00 | 21.78 |
|    | ATOM | 1177 | N   | LYS | A | 153 | 3.163  | 31.316 | 53.934 | 1.00 | 21.69 |
|    | ATOM | 1178 | CA  | LYS | A | 153 | 4.146  | 31.985 | 53.101 | 1.00 | 20.64 |
|    | ATOM | 1179 | C   | LYS | A | 153 | 3.606  | 32.223 | 51.720 | 1.00 | 25.15 |
| 35 | ATOM | 1180 | O   | LYS | A | 153 | 3.041  | 31.329 | 51.114 | 1.00 | 27.06 |
|    | ATOM | 1181 | CB  | LYS | A | 153 | 5.455  | 31.218 | 53.016 | 1.00 | 24.18 |
|    | ATOM | 1182 | CG  | LYS | A | 153 | 6.159  | 31.061 | 54.360 | 1.00 | 29.97 |
|    | ATOM | 1183 | CD  | LYS | A | 153 | 7.582  | 30.546 | 54.220 | 1.00 | 19.10 |
|    | ATOM | 1184 | CE  | LYS | A | 153 | 8.276  | 30.287 | 55.546 | 1.00 | 24.45 |
| 40 | ATOM | 1185 | NZ  | LYS | A | 153 | 9.760  | 30.289 | 55.457 | 1.00 | 21.92 |
|    | ATOM | 1186 | N   | LEU | A | 154 | 3.768  | 33.438 | 51.213 | 1.00 | 22.90 |
|    | ATOM | 1187 | CA  | LEU | A | 154 | 3.286  | 33.772 | 49.876 | 1.00 | 22.75 |
|    | ATOM | 1188 | C   | LEU | A | 154 | 4.280  | 34.594 | 49.091 | 1.00 | 23.26 |
|    | ATOM | 1189 | O   | LEU | A | 154 | 5.225  | 35.207 | 49.624 | 1.00 | 21.95 |
| 45 | ATOM | 1190 | CB  | LEU | A | 154 | 1.989  | 34.615 | 49.972 | 1.00 | 23.48 |
|    | ATOM | 1191 | CG  | LEU | A | 154 | 2.246  | 35.948 | 50.729 | 1.00 | 29.06 |
|    | ATOM | 1192 | CD1 | LEU | A | 154 | 1.385  | 37.086 | 50.200 | 1.00 | 29.05 |
|    | ATOM | 1193 | CD2 | LEU | A | 154 | 1.986  | 35.788 | 52.225 | 1.00 | 26.55 |
|    | ATOM | 1194 | N   | THR | A | 155 | 4.033  | 34.653 | 47.791 | 1.00 | 22.63 |
| 50 | ATOM | 1195 | CA  | THR | A | 155 | 4.862  | 35.499 | 46.940 | 1.00 | 25.54 |
|    | ATOM | 1196 | C   | THR | A | 155 | 4.088  | 36.820 | 46.772 | 1.00 | 26.35 |
|    | ATOM | 1197 | O   | THR | A | 155 | 2.929  | 36.943 | 47.190 | 1.00 | 25.33 |
|    | ATOM | 1198 | CB  | THR | A | 155 | 5.122  | 34.931 | 45.526 | 1.00 | 26.50 |
|    | ATOM | 1199 | OG1 | THR | A | 155 | 3.937  | 34.294 | 45.141 | 1.00 | 31.87 |
| 55 | ATOM | 1200 | CG2 | THR | A | 155 | 6.327  | 33.991 | 45.488 | 1.00 | 21.48 |
|    | ATOM | 1201 | N   | TYR | A | 156 | 4.721  | 37.802 | 46.154 | 1.00 | 23.09 |
|    | ATOM | 1202 | CA  | TYR | A | 156 | 4.021  | 39.040 | 45.943 | 1.00 | 22.25 |
|    | ATOM | 1203 | C   | TYR | A | 156 | 4.631  | 39.924 | 44.889 | 1.00 | 24.76 |
|    | ATOM | 1204 | O   | TYR | A | 156 | 5.846  | 39.919 | 44.601 | 1.00 | 28.65 |
| 60 | ATOM | 1205 | CB  | TYR | A | 156 | 3.735  | 39.831 | 47.252 | 1.00 | 22.99 |
|    | ATOM | 1206 | CG  | TYR | A | 156 | 4.853  | 40.754 | 47.751 | 1.00 | 24.46 |
|    | ATOM | 1207 | CD1 | TYR | A | 156 | 4.992  | 42.048 | 47.246 | 1.00 | 26.47 |
|    | ATOM | 1208 | CD2 | TYR | A | 156 | 5.744  | 40.356 | 48.755 | 1.00 | 22.08 |
|    | ATOM | 1209 | CE1 | TYR | A | 156 | 6.003  | 42.894 | 47.704 | 1.00 | 27.20 |
|    | ATOM | 1210 | CE2 | TYR | A | 156 | 6.755  | 41.194 | 49.242 | 1.00 | 19.36 |



|    |      |      |     |           |        |        |        |      |        |
|----|------|------|-----|-----------|--------|--------|--------|------|--------|
|    | ATOM | 1211 | CZ  | TYR A 156 | 6.874  | 42.476 | 48.709 | 1.00 | 28.26  |
|    | ATOM | 1212 | OH  | TYR A 156 | 7.819  | 43.341 | 49.176 | 1.00 | 23.92  |
|    | ATOM | 1213 | N   | THR A 157 | 3.737  | 40.711 | 44.325 | 1.00 | 20.53  |
|    | ATOM | 1214 | CA  | THR A 157 | 4.079  | 41.726 | 43.358 | 1.00 | 22.66  |
| 5  | ATOM | 1215 | C   | THR A 157 | 3.374  | 42.996 | 43.844 | 1.00 | 27.95  |
|    | ATOM | 1216 | O   | THR A 157 | 2.300  | 42.941 | 44.469 | 1.00 | 27.60  |
|    | ATOM | 1217 | CB  | THR A 157 | 3.660  | 41.345 | 41.931 | 1.00 | 36.12  |
|    | ATOM | 1218 | OG1 | THR A 157 | 2.311  | 40.913 | 41.927 | 1.00 | 35.88  |
|    | ATOM | 1219 | CG2 | THR A 157 | 4.528  | 40.177 | 41.502 | 1.00 | 31.47  |
| 10 | ATOM | 1220 | N   | ALA A 158 | 3.984  | 44.136 | 43.604 | 1.00 | 26.56  |
|    | ATOM | 1221 | CA  | ALA A 158 | 3.357  | 45.363 | 44.034 | 1.00 | 28.25  |
|    | ATOM | 1222 | C   | ALA A 158 | 3.661  | 46.555 | 43.115 | 1.00 | 33.79  |
|    | ATOM | 1223 | O   | ALA A 158 | 4.737  | 46.682 | 42.469 | 1.00 | 31.04  |
|    | ATOM | 1224 | CB  | ALA A 158 | 3.749  | 45.700 | 45.460 | 1.00 | 26.89  |
| 15 | ATOM | 1225 | N   | GLU A 159 | 2.693  | 47.453 | 43.081 | 1.00 | 30.94  |
|    | ATOM | 1226 | CA  | GLU A 159 | 2.863  | 48.658 | 42.328 | 1.00 | 32.37  |
|    | ATOM | 1227 | C   | GLU A 159 | 2.434  | 49.789 | 43.226 | 1.00 | 31.24  |
|    | ATOM | 1228 | O   | GLU A 159 | 1.311  | 49.803 | 43.735 | 1.00 | 29.85  |
|    | ATOM | 1229 | CB  | GLU A 159 | 2.118  | 48.680 | 40.993 | 1.00 | 35.41  |
| 20 | ATOM | 1230 | CG  | GLU A 159 | 1.749  | 47.300 | 40.444 | 1.00 | 59.87  |
|    | ATOM | 1231 | CD  | GLU A 159 | 0.983  | 47.438 | 39.160 | 1.00 | 98.76  |
|    | ATOM | 1232 | OE1 | GLU A 159 | -0.110 | 47.979 | 39.091 | 1.00 | 78.51  |
|    | ATOM | 1233 | OE2 | GLU A 159 | 1.636  | 46.958 | 38.126 | 1.00 | 100.00 |
|    | ATOM | 1234 | N   | VAL A 160 | 3.337  | 50.714 | 43.472 | 1.00 | 28.73  |
| 25 | ATOM | 1235 | CA  | VAL A 160 | 2.915  | 51.778 | 44.352 | 1.00 | 29.43  |
|    | ATOM | 1236 | C   | VAL A 160 | 3.180  | 53.148 | 43.786 | 1.00 | 29.09  |
|    | ATOM | 1237 | O   | VAL A 160 | 4.292  | 53.442 | 43.354 | 1.00 | 27.09  |
|    | ATOM | 1238 | CB  | VAL A 160 | 3.370  | 51.589 | 45.785 | 1.00 | 33.76  |
|    | ATOM | 1239 | CG1 | VAL A 160 | 4.212  | 50.321 | 45.892 | 1.00 | 33.85  |
| 30 | ATOM | 1240 | CG2 | VAL A 160 | 4.097  | 52.814 | 46.314 | 1.00 | 32.12  |
|    | ATOM | 1241 | N   | SER A 161 | 2.132  | 53.967 | 43.760 | 1.00 | 29.81  |
|    | ATOM | 1242 | CA  | SER A 161 | 2.249  | 55.323 | 43.202 | 1.00 | 29.33  |
|    | ATOM | 1243 | C   | SER A 161 | 2.558  | 56.310 | 44.299 | 1.00 | 30.68  |
|    | ATOM | 1244 | O   | SER A 161 | 1.840  | 56.364 | 45.299 | 1.00 | 32.33  |
| 35 | ATOM | 1245 | CB  | SER A 161 | 0.963  | 55.756 | 42.514 | 1.00 | 32.12  |
|    | ATOM | 1246 | OG  | SER A 161 | 1.074  | 57.091 | 42.092 | 1.00 | 36.30  |
|    | ATOM | 1247 | N   | VAL A 162 | 3.614  | 57.073 | 44.115 | 1.00 | 24.51  |
|    | ATOM | 1248 | CA  | VAL A 162 | 3.968  | 58.033 | 45.125 | 1.00 | 25.24  |
|    | ATOM | 1249 | C   | VAL A 162 | 4.187  | 59.371 | 44.477 | 1.00 | 37.10  |
| 40 | ATOM | 1250 | O   | VAL A 162 | 4.359  | 59.438 | 43.257 | 1.00 | 36.28  |
|    | ATOM | 1251 | CB  | VAL A 162 | 5.284  | 57.657 | 45.821 | 1.00 | 25.44  |
|    | ATOM | 1252 | CG1 | VAL A 162 | 5.213  | 56.287 | 46.487 | 1.00 | 24.46  |
|    | ATOM | 1253 | CG2 | VAL A 162 | 6.429  | 57.684 | 44.831 | 1.00 | 24.47  |
|    | ATOM | 1254 | N   | PRO A 163 | 4.203  | 60.416 | 45.312 | 1.00 | 31.09  |
| 45 | ATOM | 1255 | CA  | PRO A 163 | 4.476  | 61.733 | 44.805 | 1.00 | 31.84  |
|    | ATOM | 1256 | C   | PRO A 163 | 5.792  | 61.640 | 44.040 | 1.00 | 31.38  |
|    | ATOM | 1257 | O   | PRO A 163 | 6.821  | 61.177 | 44.545 | 1.00 | 30.83  |
|    | ATOM | 1258 | CB  | PRO A 163 | 4.545  | 62.640 | 46.047 | 1.00 | 33.90  |
|    | ATOM | 1259 | CG  | PRO A 163 | 3.818  | 61.891 | 47.158 | 1.00 | 36.16  |
| 50 | ATOM | 1260 | CD  | PRO A 163 | 3.635  | 60.458 | 46.680 | 1.00 | 29.11  |
|    | ATOM | 1261 | N   | LYS A 164 | 5.738  | 62.040 | 42.789 | 1.00 | 30.95  |
|    | ATOM | 1262 | CA  | LYS A 164 | 6.875  | 61.950 | 41.891 | 1.00 | 30.90  |
|    | ATOM | 1263 | C   | LYS A 164 | 8.223  | 62.361 | 42.405 | 1.00 | 32.87  |
|    | ATOM | 1264 | O   | LYS A 164 | 9.249  | 61.973 | 41.850 | 1.00 | 29.98  |
| 55 | ATOM | 1265 | CB  | LYS A 164 | 6.614  | 62.525 | 40.525 | 1.00 | 38.69  |
|    | ATOM | 1266 | CG  | LYS A 164 | 5.381  | 63.405 | 40.464 | 1.00 | 60.47  |
|    | ATOM | 1267 | CD  | LYS A 164 | 5.608  | 64.642 | 39.612 | 1.00 | 87.95  |
|    | ATOM | 1268 | CE  | LYS A 164 | 6.869  | 64.557 | 38.757 | 1.00 | 94.83  |
|    | ATOM | 1269 | NZ  | LYS A 164 | 7.762  | 65.712 | 38.926 | 1.00 | 100.00 |
| 60 | ATOM | 1270 | N   | GLU A 165 | 8.253  | 63.168 | 43.445 | 1.00 | 32.55  |
|    | ATOM | 1271 | CA  | GLU A 165 | 9.540  | 63.587 | 43.946 | 1.00 | 33.95  |
|    | ATOM | 1272 | C   | GLU A 165 | 10.107 | 62.617 | 44.949 | 1.00 | 36.46  |
|    | ATOM | 1273 | O   | GLU A 165 | 11.245 | 62.742 | 45.348 | 1.00 | 36.58  |
|    | ATOM | 1274 | CB  | GLU A 165 | 9.510  | 65.006 | 44.540 | 1.00 | 37.35  |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
|    | ATOM | 1275 | CG  | GLU | A | 165 | 8.599  | 65.165 | 45.784 | 1.00 | 53.54 |
|    | ATOM | 1276 | CD  | GLU | A | 165 | 7.138  | 65.409 | 45.480 | 1.00 | 77.59 |
|    | ATOM | 1277 | OE1 | GLU | A | 165 | 6.598  | 65.114 | 44.421 | 1.00 | 44.13 |
| 5  | ATOM | 1278 | OE2 | GLU | A | 165 | 6.512  | 65.959 | 46.494 | 1.00 | 78.66 |
|    | ATOM | 1279 | N   | LEU | A | 166 | 9.314  | 61.641 | 45.318 | 1.00 | 33.08 |
|    | ATOM | 1280 | CA  | LEU | A | 166 | 9.772  | 60.695 | 46.299 | 1.00 | 33.49 |
|    | ATOM | 1281 | C   | LEU | A | 166 | 10.068 | 59.321 | 45.734 | 1.00 | 40.05 |
|    | ATOM | 1282 | O   | LEU | A | 166 | 9.578  | 58.987 | 44.646 | 1.00 | 41.96 |
| 10 | ATOM | 1283 | CB  | LEU | A | 166 | 8.727  | 60.596 | 47.423 | 1.00 | 31.45 |
|    | ATOM | 1284 | CG  | LEU | A | 166 | 8.352  | 61.938 | 48.020 | 1.00 | 29.81 |
|    | ATOM | 1285 | CD1 | LEU | A | 166 | 7.242  | 61.711 | 49.041 | 1.00 | 27.01 |
|    | ATOM | 1286 | CD2 | LEU | A | 166 | 9.598  | 62.582 | 48.632 | 1.00 | 21.37 |
|    | ATOM | 1287 | N   | VAL | A | 167 | 10.874 | 58.544 | 46.500 | 1.00 | 30.67 |
| 15 | ATOM | 1288 | CA  | VAL | A | 167 | 11.238 | 57.178 | 46.138 | 1.00 | 29.31 |
|    | ATOM | 1289 | C   | VAL | A | 167 | 10.478 | 56.157 | 46.996 | 1.00 | 35.64 |
|    | ATOM | 1290 | O   | VAL | A | 167 | 10.216 | 56.385 | 48.183 | 1.00 | 32.65 |
|    | ATOM | 1291 | CB  | VAL | A | 167 | 12.721 | 56.904 | 46.304 | 1.00 | 30.60 |
|    | ATOM | 1292 | CG1 | VAL | A | 167 | 13.000 | 55.483 | 45.849 | 1.00 | 29.30 |
|    | ATOM | 1293 | CG2 | VAL | A | 167 | 13.562 | 57.880 | 45.521 | 1.00 | 31.04 |
| 20 | ATOM | 1294 | N   | ALA | A | 168 | 10.132 | 55.017 | 46.400 | 1.00 | 33.01 |
|    | ATOM | 1295 | CA  | ALA | A | 168 | 9.453  | 53.943 | 47.115 | 1.00 | 29.38 |
|    | ATOM | 1296 | C   | ALA | A | 168 | 10.289 | 52.685 | 46.978 | 1.00 | 36.90 |
|    | ATOM | 1297 | O   | ALA | A | 168 | 10.786 | 52.362 | 45.875 | 1.00 | 37.97 |
| 25 | ATOM | 1298 | CB  | ALA | A | 168 | 8.046  | 53.694 | 46.637 | 1.00 | 28.00 |
|    | ATOM | 1299 | N   | LEU | A | 169 | 10.482 | 51.997 | 48.110 | 1.00 | 28.52 |
|    | ATOM | 1300 | CA  | LEU | A | 169 | 11.256 | 50.769 | 48.139 | 1.00 | 24.26 |
|    | ATOM | 1301 | C   | LEU | A | 169 | 10.464 | 49.738 | 48.879 | 1.00 | 27.24 |
|    | ATOM | 1302 | O   | LEU | A | 169 | 9.694  | 50.071 | 49.786 | 1.00 | 25.74 |
| 30 | ATOM | 1303 | CB  | LEU | A | 169 | 12.615 | 50.908 | 48.841 | 1.00 | 24.31 |
|    | ATOM | 1304 | CG  | LEU | A | 169 | 13.525 | 51.974 | 48.250 | 1.00 | 28.56 |
|    | ATOM | 1305 | CD1 | LEU | A | 169 | 14.739 | 52.181 | 49.173 | 1.00 | 27.05 |
|    | ATOM | 1306 | CD2 | LEU | A | 169 | 13.993 | 51.550 | 46.852 | 1.00 | 27.25 |
|    | ATOM | 1307 | N   | MET | A | 170 | 10.649 | 48.480 | 48.486 | 1.00 | 26.02 |
| 35 | ATOM | 1308 | CA  | MET | A | 170 | 9.952  | 47.392 | 49.144 | 1.00 | 23.03 |
|    | ATOM | 1309 | C   | MET | A | 170 | 10.856 | 46.224 | 49.455 | 1.00 | 18.57 |
|    | ATOM | 1310 | O   | MET | A | 170 | 12.033 | 46.212 | 49.085 | 1.00 | 20.77 |
|    | ATOM | 1311 | CB  | MET | A | 170 | 8.712  | 46.943 | 48.371 | 1.00 | 24.60 |
|    | ATOM | 1312 | CG  | MET | A | 170 | 7.654  | 47.979 | 48.535 | 1.00 | 25.34 |
| 40 | ATOM | 1313 | SD  | MET | A | 170 | 6.105  | 47.419 | 47.869 | 1.00 | 28.58 |
|    | ATOM | 1314 | CE  | MET | A | 170 | 5.380  | 46.463 | 49.232 | 1.00 | 24.66 |
|    | ATOM | 1315 | N   | SER | A | 171 | 10.298 | 45.244 | 50.173 | 1.00 | 17.78 |
|    | ATOM | 1316 | CA  | SER | A | 171 | 11.062 | 44.069 | 50.482 | 1.00 | 16.80 |
|    | ATOM | 1317 | C   | SER | A | 171 | 10.905 | 43.128 | 49.265 | 1.00 | 26.03 |
| 45 | ATOM | 1318 | O   | SER | A | 171 | 10.389 | 42.018 | 49.344 | 1.00 | 25.31 |
|    | ATOM | 1319 | CB  | SER | A | 171 | 10.527 | 43.436 | 51.748 | 1.00 | 17.00 |
|    | ATOM | 1320 | OG  | SER | A | 171 | 9.130  | 43.207 | 51.625 | 1.00 | 20.17 |
|    | ATOM | 1321 | N   | ALA | A | 172 | 11.298 | 43.612 | 48.095 | 1.00 | 26.60 |
|    | ATOM | 1322 | CA  | ALA | A | 172 | 11.154 | 42.849 | 46.875 | 1.00 | 25.77 |
| 50 | ATOM | 1323 | C   | ALA | A | 172 | 12.153 | 43.339 | 45.860 | 1.00 | 32.28 |
|    | ATOM | 1324 | O   | ALA | A | 172 | 12.897 | 44.299 | 46.114 | 1.00 | 26.87 |
|    | ATOM | 1325 | CB  | ALA | A | 172 | 9.762  | 43.083 | 46.332 | 1.00 | 25.21 |
|    | ATOM | 1326 | N   | ILE | A | 173 | 12.180 | 42.678 | 44.700 | 1.00 | 30.44 |
|    | ATOM | 1327 | CA  | ILE | A | 173 | 13.107 | 43.110 | 43.661 | 1.00 | 29.54 |
| 55 | ATOM | 1328 | C   | ILE | A | 173 | 12.510 | 44.319 | 42.959 | 1.00 | 30.78 |
|    | ATOM | 1329 | O   | ILE | A | 173 | 11.331 | 44.315 | 42.583 | 1.00 | 29.32 |
|    | ATOM | 1330 | CB  | ILE | A | 173 | 13.479 | 41.997 | 42.661 | 1.00 | 31.06 |
|    | ATOM | 1331 | CG1 | ILE | A | 173 | 14.210 | 40.874 | 43.388 | 1.00 | 28.42 |
|    | ATOM | 1332 | CG2 | ILE | A | 173 | 14.431 | 42.563 | 41.617 | 1.00 | 32.58 |
|    | ATOM | 1333 | CD1 | ILE | A | 173 | 15.604 | 41.286 | 43.851 | 1.00 | 33.22 |
| 60 | ATOM | 1334 | N   | ARG | A | 174 | 13.328 | 45.356 | 42.834 | 1.00 | 31.92 |
|    | ATOM | 1335 | CA  | ARG | A | 174 | 12.906 | 46.595 | 42.197 | 1.00 | 33.87 |
|    | ATOM | 1336 | C   | ARG | A | 174 | 12.582 | 46.236 | 40.785 | 1.00 | 39.44 |
|    | ATOM | 1337 | O   | ARG | A | 174 | 13.467 | 45.775 | 40.091 | 1.00 | 34.80 |
|    | ATOM | 1338 | CB  | ARG | A | 174 | 14.004 | 47.669 | 42.218 | 1.00 | 35.31 |



|    |      |      |     |     |   |     |        |        |        |      |        |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
|    | ATOM | 1339 | CG  | ARG | A | 174 | 14.186 | 48.368 | 43.579 | 1.00 | 42.88  |
|    | ATOM | 1340 | CD  | ARG | A | 174 | 15.229 | 49.492 | 43.608 | 1.00 | 39.93  |
|    | ATOM | 1341 | NE  | ARG | A | 174 | 16.516 | 49.129 | 43.013 | 1.00 | 59.20  |
| 5  | ATOM | 1342 | CZ  | ARG | A | 174 | 17.329 | 49.992 | 42.407 | 1.00 | 92.36  |
|    | ATOM | 1343 | NH1 | ARG | A | 174 | 17.032 | 51.288 | 42.284 | 1.00 | 100.00 |
|    | ATOM | 1344 | NH2 | ARG | A | 174 | 18.474 | 49.542 | 41.901 | 1.00 | 84.94  |
|    | ATOM | 1345 | N   | ASP | A | 175 | 11.324 | 46.397 | 40.406 | 1.00 | 44.29  |
|    | ATOM | 1346 | CA  | ASP | A | 175 | 10.850 | 46.070 | 39.076 | 1.00 | 48.46  |
| 10 | ATOM | 1347 | C   | ASP | A | 175 | 10.987 | 47.236 | 38.107 | 1.00 | 61.94  |
|    | ATOM | 1348 | O   | ASP | A | 175 | 11.709 | 47.177 | 37.124 | 1.00 | 69.21  |
|    | ATOM | 1349 | CB  | ASP | A | 175 | 9.401  | 45.553 | 39.111 | 1.00 | 52.28  |
|    | ATOM | 1350 | CG  | ASP | A | 175 | 9.079  | 44.536 | 38.041 | 1.00 | 76.56  |
|    | ATOM | 1351 | OD1 | ASP | A | 175 | 9.926  | 44.028 | 37.313 | 1.00 | 76.21  |
| 15 | ATOM | 1352 | OD2 | ASP | A | 175 | 7.788  | 44.270 | 37.964 | 1.00 | 85.33  |
|    | ATOM | 1353 | N   | GLY | A | 176 | 10.293 | 48.309 | 38.369 | 1.00 | 59.49  |
|    | ATOM | 1354 | CA  | GLY | A | 176 | 10.405 | 49.442 | 37.489 | 1.00 | 59.25  |
|    | ATOM | 1355 | C   | GLY | A | 176 | 9.723  | 50.662 | 38.055 | 1.00 | 62.28  |
|    | ATOM | 1356 | O   | GLY | A | 176 | 8.958  | 50.585 | 39.026 | 1.00 | 61.93  |
| 20 | ATOM | 1357 | N   | GLU | A | 177 | 10.028 | 51.784 | 37.418 | 1.00 | 56.86  |
|    | ATOM | 1358 | CA  | GLU | A | 177 | 9.473  | 53.070 | 37.772 | 1.00 | 56.20  |
|    | ATOM | 1359 | C   | GLU | A | 177 | 9.128  | 53.804 | 36.495 | 1.00 | 66.31  |
|    | ATOM | 1360 | O   | GLU | A | 177 | 9.865  | 53.745 | 35.499 | 1.00 | 67.90  |
|    | ATOM | 1361 | CB  | GLU | A | 177 | 10.411 | 53.926 | 38.645 | 1.00 | 55.46  |
| 25 | ATOM | 1362 | CG  | GLU | A | 177 | 11.304 | 54.835 | 37.783 | 1.00 | 54.29  |
|    | ATOM | 1363 | CD  | GLU | A | 177 | 11.996 | 55.940 | 38.534 | 1.00 | 73.05  |
|    | ATOM | 1364 | OE1 | GLU | A | 177 | 11.471 | 57.005 | 38.805 | 1.00 | 66.34  |
|    | ATOM | 1365 | OE2 | GLU | A | 177 | 13.242 | 55.657 | 38.817 | 1.00 | 54.79  |
|    | ATOM | 1366 | N   | THR | A | 178 | 7.997  | 54.483 | 36.541 | 1.00 | 63.56  |
| 30 | ATOM | 1367 | CA  | THR | A | 178 | 7.496  | 55.245 | 35.419 | 1.00 | 63.49  |
|    | ATOM | 1368 | C   | THR | A | 178 | 6.534  | 56.305 | 35.923 | 1.00 | 64.39  |
|    | ATOM | 1369 | O   | THR | A | 178 | 6.338  | 56.452 | 37.118 | 1.00 | 65.55  |
|    | ATOM | 1370 | CB  | THR | A | 178 | 6.737  | 54.290 | 34.479 | 1.00 | 79.55  |
|    | ATOM | 1371 | OG1 | THR | A | 178 | 6.206  | 55.012 | 33.376 | 1.00 | 100.00 |
| 35 | ATOM | 1372 | CG2 | THR | A | 178 | 5.617  | 53.590 | 35.263 | 1.00 | 62.95  |
|    | ATOM | 1373 | N   | PRO | A | 179 | 5.919  | 57.042 | 35.013 | 1.00 | 56.32  |
|    | ATOM | 1374 | CA  | PRO | A | 179 | 4.958  | 58.025 | 35.406 | 1.00 | 51.92  |
|    | ATOM | 1375 | C   | PRO | A | 179 | 3.593  | 57.388 | 35.536 | 1.00 | 51.24  |
|    | ATOM | 1376 | O   | PRO | A | 179 | 3.192  | 56.586 | 34.698 | 1.00 | 51.46  |
| 40 | ATOM | 1377 | CB  | PRO | A | 179 | 4.942  | 59.054 | 34.282 | 1.00 | 53.51  |
|    | ATOM | 1378 | CG  | PRO | A | 179 | 6.214  | 58.838 | 33.470 | 1.00 | 59.43  |
|    | ATOM | 1379 | CD  | PRO | A | 179 | 6.905  | 57.628 | 34.060 | 1.00 | 56.49  |
|    | ATOM | 1380 | N   | ASP | A | 180 | 2.906  | 57.739 | 36.614 | 1.00 | 44.92  |
|    | ATOM | 1381 | CA  | ASP | A | 180 | 1.581  | 57.264 | 36.884 | 1.00 | 45.28  |
| 45 | ATOM | 1382 | C   | ASP | A | 180 | 0.780  | 57.912 | 35.799 | 1.00 | 62.22  |
|    | ATOM | 1383 | O   | ASP | A | 180 | 1.131  | 59.004 | 35.376 | 1.00 | 62.62  |
|    | ATOM | 1384 | CB  | ASP | A | 180 | 1.156  | 57.806 | 38.255 | 1.00 | 43.41  |
|    | ATOM | 1385 | CG  | ASP | A | 180 | -0.212 | 57.380 | 38.679 | 1.00 | 48.40  |
|    | ATOM | 1386 | OD1 | ASP | A | 180 | -1.073 | 56.997 | 37.904 | 1.00 | 53.37  |
| 50 | ATOM | 1387 | OD2 | ASP | A | 180 | -0.383 | 57.463 | 39.973 | 1.00 | 47.57  |
|    | ATOM | 1388 | N   | PRO | A | 181 | -0.243 | 57.280 | 35.296 | 1.00 | 69.44  |
|    | ATOM | 1389 | CA  | PRO | A | 181 | -0.950 | 57.955 | 34.234 | 1.00 | 72.53  |
|    | ATOM | 1390 | C   | PRO | A | 181 | -2.382 | 58.272 | 34.587 | 1.00 | 82.99  |
|    | ATOM | 1391 | O   | PRO | A | 181 | -3.231 | 58.459 | 33.717 | 1.00 | 84.95  |
| 55 | ATOM | 1392 | CB  | PRO | A | 181 | -0.829 | 57.076 | 32.987 | 1.00 | 74.39  |
|    | ATOM | 1393 | CG  | PRO | A | 181 | 0.153  | 55.954 | 33.319 | 1.00 | 77.89  |
|    | ATOM | 1394 | CD  | PRO | A | 181 | 0.458  | 56.057 | 34.810 | 1.00 | 71.93  |
|    | ATOM | 1395 | N   | GLU | A | 182 | -2.632 | 58.382 | 35.887 | 1.00 | 83.47  |
|    | ATOM | 1396 | CA  | GLU | A | 182 | -3.961 | 58.676 | 36.386 | 1.00 | 86.24  |
| 60 | ATOM | 1397 | C   | GLU | A | 182 | -4.259 | 60.167 | 36.436 | 1.00 | 98.16  |
|    | ATOM | 1398 | O   | GLU | A | 182 | -4.003 | 60.882 | 35.460 | 1.00 | 100.00 |
|    | ATOM | 1399 | CB  | GLU | A | 182 | -4.278 | 57.994 | 37.726 | 1.00 | 87.28  |
|    | ATOM | 1400 | CG  | GLU | A | 182 | -5.779 | 57.681 | 37.863 | 1.00 | 90.17  |
|    | ATOM | 1401 | CD  | GLU | A | 182 | -6.257 | 56.682 | 36.842 | 1.00 | 100.00 |
|    | ATOM | 1402 | OE1 | GLU | A | 182 | -6.233 | 56.882 | 35.637 | 1.00 | 100.00 |



|    |      |      |     |     |   |     |        |        |        |            |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------------|
|    | ATOM | 1403 | OE2 | GLU | A | 182 | -6.718 | 55.578 | 37.385 | 1.00100.00 |
|    | ATOM | 1404 | N   | ASP | A | 183 | -4.767 | 60.640 | 37.598 | 1.00 96.59 |
|    | ATOM | 1405 | CA  | ASP | A | 183 | -5.124 | 62.060 | 37.848 | 1.00 97.69 |
| 5  | ATOM | 1406 | C   | ASP | A | 183 | -4.078 | 62.809 | 38.721 | 1.00100.00 |
|    | ATOM | 1407 | O   | ASP | A | 183 | -4.439 | 63.829 | 39.375 | 1.00100.00 |
|    | ATOM | 1408 | CB  | ASP | A | 183 | -6.477 | 62.127 | 38.653 | 1.00 99.62 |
|    | ATOM | 1409 | CG  | ASP | A | 183 | -7.712 | 61.432 | 38.090 | 1.00100.00 |
|    | ATOM | 1410 | OD1 | ASP | A | 183 | -8.310 | 60.544 | 38.680 | 1.00100.00 |
| 10 | ATOM | 1411 | OD2 | ASP | A | 183 | -8.091 | 61.903 | 36.918 | 1.00100.00 |
|    | ATOM | 1412 | N   | PRO | A | 184 | -2.797 | 62.341 | 38.750 | 1.00 95.70 |
|    | ATOM | 1413 | CA  | PRO | A | 184 | -1.734 | 62.796 | 39.641 | 1.00 94.16 |
|    | ATOM | 1414 | C   | PRO | A | 184 | -0.516 | 63.593 | 39.206 | 1.00 96.46 |
|    | ATOM | 1415 | O   | PRO | A | 184 | -0.294 | 63.958 | 38.050 | 1.00 99.66 |
| 15 | ATOM | 1416 | CB  | PRO | A | 184 | -0.980 | 61.479 | 39.654 | 1.00 95.77 |
|    | ATOM | 1417 | CG  | PRO | A | 184 | -0.835 | 61.166 | 38.163 | 1.00 99.25 |
|    | ATOM | 1418 | CD  | PRO | A | 184 | -2.085 | 61.763 | 37.565 | 1.00 94.91 |
|    | ATOM | 1419 | N   | SER | A | 185 | 0.318  | 63.703 | 40.258 | 1.00 86.69 |
|    | ATOM | 1420 | CA  | SER | A | 185 | 1.658  | 64.262 | 40.362 | 1.00 82.33 |
| 20 | ATOM | 1421 | C   | SER | A | 185 | 2.434  | 63.253 | 41.219 | 1.00 77.73 |
|    | ATOM | 1422 | O   | SER | A | 185 | 3.198  | 63.570 | 42.144 | 1.00 79.49 |
|    | ATOM | 1423 | CB  | SER | A | 185 | 1.710  | 65.661 | 40.921 | 1.00 85.04 |
|    | ATOM | 1424 | OG  | SER | A | 185 | 2.756  | 66.349 | 40.263 | 1.00 97.98 |
|    | ATOM | 1425 | N   | ARG | A | 186 | 2.121  | 61.994 | 40.856 | 1.00 62.61 |
| 25 | ATOM | 1426 | CA  | ARG | A | 186 | 2.591  | 60.741 | 41.404 | 1.00 55.55 |
|    | ATOM | 1427 | C   | ARG | A | 186 | 3.444  | 59.990 | 40.366 | 1.00 56.85 |
|    | ATOM | 1428 | O   | ARG | A | 186 | 3.354  | 60.216 | 39.158 | 1.00 56.42 |
|    | ATOM | 1429 | CB  | ARG | A | 186 | 1.388  | 59.859 | 41.742 | 1.00 41.52 |
|    | ATOM | 1430 | CG  | ARG | A | 186 | 0.432  | 60.389 | 42.805 | 1.00 32.21 |
| 30 | ATOM | 1431 | CD  | ARG | A | 186 | 0.602  | 59.683 | 44.153 | 1.00 42.93 |
|    | ATOM | 1432 | NE  | ARG | A | 186 | -0.519 | 59.935 | 45.043 | 1.00 79.86 |
|    | ATOM | 1433 | CZ  | ARG | A | 186 | -0.467 | 60.731 | 46.113 | 1.00100.00 |
|    | ATOM | 1434 | NH1 | ARG | A | 186 | 0.659  | 61.360 | 46.468 | 1.00100.00 |
|    | ATOM | 1435 | NH2 | ARG | A | 186 | -1.566 | 60.880 | 46.860 | 1.00100.00 |
| 35 | ATOM | 1436 | N   | LYS | A | 187 | 4.273  | 59.078 | 40.867 | 1.00 47.78 |
|    | ATOM | 1437 | CA  | LYS | A | 187 | 5.164  | 58.231 | 40.095 | 1.00 44.24 |
|    | ATOM | 1438 | C   | LYS | A | 187 | 4.856  | 56.802 | 40.532 | 1.00 50.17 |
|    | ATOM | 1439 | O   | LYS | A | 187 | 4.464  | 56.573 | 41.684 | 1.00 49.60 |
|    | ATOM | 1440 | CB  | LYS | A | 187 | 6.604  | 58.608 | 40.417 | 1.00 45.31 |
| 40 | ATOM | 1441 | CG  | LYS | A | 187 | 7.703  | 57.832 | 39.706 | 1.00 37.40 |
|    | ATOM | 1442 | CD  | LYS | A | 187 | 9.099  | 58.045 | 40.318 | 1.00 37.61 |
|    | ATOM | 1443 | CE  | LYS | A | 187 | 9.919  | 59.196 | 39.732 | 1.00 27.19 |
|    | ATOM | 1444 | NZ  | LYS | A | 187 | 11.371 | 59.057 | 39.898 | 1.00 40.78 |
|    | ATOM | 1445 | N   | ILE | A | 188 | 5.006  | 55.832 | 39.620 | 1.00 46.34 |
| 45 | ATOM | 1446 | CA  | ILE | A | 188 | 4.732  | 54.438 | 39.963 | 1.00 43.89 |
|    | ATOM | 1447 | C   | ILE | A | 188 | 5.884  | 53.438 | 40.044 | 1.00 45.27 |
|    | ATOM | 1448 | O   | ILE | A | 188 | 6.596  | 53.147 | 39.068 | 1.00 42.03 |
|    | ATOM | 1449 | CB  | ILE | A | 188 | 3.357  | 53.861 | 39.782 | 1.00 46.49 |
|    | ATOM | 1450 | CG1 | ILE | A | 188 | 3.571  | 52.427 | 39.378 | 1.00 46.61 |
| 50 | ATOM | 1451 | CG2 | ILE | A | 188 | 2.528  | 54.603 | 38.744 | 1.00 45.69 |
|    | ATOM | 1452 | CD1 | ILE | A | 188 | 2.888  | 51.492 | 40.354 | 1.00 66.60 |
|    | ATOM | 1453 | N   | TYR | A | 189 | 6.055  | 52.933 | 41.277 | 1.00 39.79 |
|    | ATOM | 1454 | CA  | TYR | A | 189 | 7.108  | 52.024 | 41.630 | 1.00 36.01 |
|    | ATOM | 1455 | C   | TYR | A | 189 | 6.634  | 50.615 | 41.665 | 1.00 36.02 |
| 55 | ATOM | 1456 | O   | TYR | A | 189 | 5.632  | 50.291 | 42.321 | 1.00 36.41 |
|    | ATOM | 1457 | CB  | TYR | A | 189 | 7.766  | 52.446 | 42.952 | 1.00 37.07 |
|    | ATOM | 1458 | CG  | TYR | A | 189 | 8.644  | 53.677 | 42.783 | 1.00 36.77 |
|    | ATOM | 1459 | CD1 | TYR | A | 189 | 9.904  | 53.567 | 42.197 | 1.00 39.01 |
|    | ATOM | 1460 | CD2 | TYR | A | 189 | 8.216  | 54.942 | 43.193 | 1.00 34.62 |
| 60 | ATOM | 1461 | CE1 | TYR | A | 189 | 10.733 | 54.675 | 42.029 | 1.00 41.28 |
|    | ATOM | 1462 | CE2 | TYR | A | 189 | 9.023  | 56.067 | 43.031 | 1.00 33.53 |
|    | ATOM | 1463 | CZ  | TYR | A | 189 | 10.279 | 55.927 | 42.441 | 1.00 44.38 |
|    | ATOM | 1464 | OH  | TYR | A | 189 | 11.084 | 57.022 | 42.277 | 1.00 44.92 |
|    | ATOM | 1465 | N   | LYS | A | 190 | 7.395  | 49.801 | 40.929 | 1.00 35.47 |
|    | ATOM | 1466 | CA  | LYS | A | 190 | 7.125  | 48.373 | 40.772 | 1.00 36.67 |



|    |      |      |     |     |   |     |        |        |        |      |       |
|----|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
|    | ATOM | 1467 | C   | LYS | A | 190 | 8.131  | 47.441 | 41.475 | 1.00 | 32.16 |
|    | ATOM | 1468 | O   | LYS | A | 190 | 9.337  | 47.667 | 41.471 | 1.00 | 30.99 |
|    | ATOM | 1469 | CB  | LYS | A | 190 | 6.872  | 47.992 | 39.310 | 1.00 | 39.45 |
| 5  | ATOM | 1470 | CG  | LYS | A | 190 | 5.457  | 48.328 | 38.833 | 1.00 | 44.38 |
|    | ATOM | 1471 | CD  | LYS | A | 190 | 5.417  | 49.126 | 37.539 | 1.00 | 56.65 |
|    | ATOM | 1472 | CE  | LYS | A | 190 | 5.539  | 48.274 | 36.282 | 1.00 | 73.04 |
|    | ATOM | 1473 | NZ  | LYS | A | 190 | 6.686  | 48.658 | 35.433 | 1.00 | 92.77 |
|    | ATOM | 1474 | N   | PHE | A | 191 | 7.592  | 46.380 | 42.076 | 1.00 | 27.93 |
| 10 | ATOM | 1475 | CA  | PHE | A | 191 | 8.393  | 45.421 | 42.812 | 1.00 | 25.63 |
|    | ATOM | 1476 | C   | PHE | A | 191 | 7.916  | 43.986 | 42.679 | 1.00 | 25.33 |
|    | ATOM | 1477 | O   | PHE | A | 191 | 6.708  | 43.667 | 42.633 | 1.00 | 24.55 |
|    | ATOM | 1478 | CB  | PHE | A | 191 | 8.281  | 45.779 | 44.306 | 1.00 | 27.49 |
|    | ATOM | 1479 | CG  | PHE | A | 191 | 8.548  | 47.238 | 44.618 | 1.00 | 26.47 |
| 15 | ATOM | 1480 | CD1 | PHE | A | 191 | 9.838  | 47.668 | 44.922 | 1.00 | 27.21 |
|    | ATOM | 1481 | CD2 | PHE | A | 191 | 7.508  | 48.167 | 44.619 | 1.00 | 27.67 |
|    | ATOM | 1482 | CE1 | PHE | A | 191 | 10.086 | 49.004 | 45.223 | 1.00 | 28.50 |
|    | ATOM | 1483 | CE2 | PHE | A | 191 | 7.739  | 49.510 | 44.909 | 1.00 | 29.86 |
|    | ATOM | 1484 | CZ  | PHE | A | 191 | 9.038  | 49.923 | 45.205 | 1.00 | 28.47 |
| 20 | ATOM | 1485 | N   | ILE | A | 192 | 8.868  | 43.076 | 42.700 | 1.00 | 26.53 |
|    | ATOM | 1486 | CA  | ILE | A | 192 | 8.485  | 41.669 | 42.616 | 1.00 | 30.09 |
|    | ATOM | 1487 | C   | ILE | A | 192 | 9.228  | 40.779 | 43.609 | 1.00 | 26.87 |
|    | ATOM | 1488 | O   | ILE | A | 192 | 10.446 | 40.810 | 43.711 | 1.00 | 23.15 |
|    | ATOM | 1489 | CB  | ILE | A | 192 | 8.661  | 41.088 | 41.208 | 1.00 | 36.97 |
|    | ATOM | 1490 | CG1 | ILE | A | 192 | 10.132 | 40.970 | 40.936 | 1.00 | 39.49 |
| 25 | ATOM | 1491 | CG2 | ILE | A | 192 | 8.036  | 41.938 | 40.104 | 1.00 | 38.69 |
|    | ATOM | 1492 | CD1 | ILE | A | 192 | 10.620 | 39.563 | 41.245 | 1.00 | 73.45 |
|    | ATOM | 1493 | N   | GLN | A | 193 | 8.481  | 39.967 | 44.331 | 1.00 | 25.43 |
|    | ATOM | 1494 | CA  | GLN | A | 193 | 9.095  | 39.055 | 45.295 | 1.00 | 24.94 |
| 30 | ATOM | 1495 | C   | GLN | A | 193 | 8.684  | 37.626 | 44.993 | 1.00 | 25.94 |
|    | ATOM | 1496 | O   | GLN | A | 193 | 7.590  | 37.181 | 45.376 | 1.00 | 25.03 |
|    | ATOM | 1497 | CB  | GLN | A | 193 | 8.808  | 39.412 | 46.772 | 1.00 | 24.11 |
|    | ATOM | 1498 | CG  | GLN | A | 193 | 9.426  | 38.422 | 47.782 | 1.00 | 17.67 |
|    | ATOM | 1499 | CD  | GLN | A | 193 | 10.947 | 38.402 | 47.777 | 1.00 | 23.92 |
| 35 | ATOM | 1500 | OE1 | GLN | A | 193 | 11.568 | 37.485 | 47.248 | 1.00 | 24.84 |
|    | ATOM | 1501 | NE2 | GLN | A | 193 | 11.568 | 39.376 | 48.394 | 1.00 | 21.35 |
|    | ATOM | 1502 | N   | LYS | A | 194 | 9.611  | 36.945 | 44.296 | 1.00 | 24.59 |
|    | ATOM | 1503 | CA  | LYS | A | 194 | 9.486  | 35.548 | 43.842 | 1.00 | 26.30 |
|    | ATOM | 1504 | C   | LYS | A | 194 | 9.677  | 34.457 | 44.943 | 1.00 | 33.55 |
| 40 | ATOM | 1505 | O   | LYS | A | 194 | 9.254  | 33.305 | 44.759 | 1.00 | 33.23 |
|    | ATOM | 1506 | CB  | LYS | A | 194 | 10.379 | 35.289 | 42.612 | 1.00 | 26.74 |
|    | ATOM | 1507 | CG  | LYS | A | 194 | 9.722  | 35.609 | 41.258 | 1.00 | 39.96 |
|    | ATOM | 1508 | CD  | LYS | A | 194 | 10.697 | 36.137 | 40.199 | 1.00 | 47.00 |
|    | ATOM | 1509 | CE  | LYS | A | 194 | 10.182 | 36.110 | 38.751 | 1.00 | 59.13 |
| 45 | ATOM | 1510 | NZ  | LYS | A | 194 | 11.226 | 35.798 | 37.746 | 1.00 | 54.07 |
|    | ATOM | 1511 | N   | VAL | A | 195 | 10.332 | 34.795 | 46.076 | 1.00 | 25.61 |
|    | ATOM | 1512 | CA  | VAL | A | 195 | 10.542 | 33.829 | 47.155 | 1.00 | 23.02 |
|    | ATOM | 1513 | C   | VAL | A | 195 | 9.385  | 33.947 | 48.108 | 1.00 | 27.87 |
|    | ATOM | 1514 | O   | VAL | A | 195 | 9.099  | 35.029 | 48.566 | 1.00 | 29.77 |
| 50 | ATOM | 1515 | CB  | VAL | A | 195 | 11.833 | 34.049 | 47.930 | 1.00 | 22.42 |
|    | ATOM | 1516 | CG1 | VAL | A | 195 | 11.997 | 32.891 | 48.881 | 1.00 | 22.09 |
|    | ATOM | 1517 | CG2 | VAL | A | 195 | 13.057 | 34.101 | 47.027 | 1.00 | 21.83 |
|    | ATOM | 1518 | N   | PRO | A | 196 | 8.687  | 32.867 | 48.391 | 1.00 | 24.28 |
|    | ATOM | 1519 | CA  | PRO | A | 196 | 7.572  | 32.955 | 49.297 | 1.00 | 22.68 |
| 55 | ATOM | 1520 | C   | PRO | A | 196 | 8.042  | 33.362 | 50.704 | 1.00 | 27.58 |
|    | ATOM | 1521 | O   | PRO | A | 196 | 9.027  | 32.837 | 51.244 | 1.00 | 25.38 |
|    | ATOM | 1522 | CB  | PRO | A | 196 | 6.886  | 31.588 | 49.301 | 1.00 | 24.52 |
|    | ATOM | 1523 | CG  | PRO | A | 196 | 7.686  | 30.674 | 48.397 | 1.00 | 28.81 |
|    | ATOM | 1524 | CD  | PRO | A | 196 | 8.822  | 31.497 | 47.831 | 1.00 | 24.64 |
| 60 | ATOM | 1525 | N   | ILE | A | 197 | 7.339  | 34.328 | 51.287 | 1.00 | 22.20 |
|    | ATOM | 1526 | CA  | ILE | A | 197 | 7.713  | 34.810 | 52.578 | 1.00 | 19.62 |
|    | ATOM | 1527 | C   | ILE | A | 197 | 6.498  | 35.005 | 53.418 | 1.00 | 24.85 |
|    | ATOM | 1528 | O   | ILE | A | 197 | 5.391  | 35.163 | 52.919 | 1.00 | 20.49 |
|    | ATOM | 1529 | CB  | ILE | A | 197 | 8.307  | 36.176 | 52.383 | 1.00 | 21.90 |
|    | ATOM | 1530 | CG1 | ILE | A | 197 | 7.317  | 36.930 | 51.510 | 1.00 | 23.26 |







PA 240106

REC'D 29 MAY 2000

WIPO

PCT

9

# THE UNITED STATES OF AMERICA

TO ALL TO WHOM THESE PRESENTS SHALL COME:

UNITED STATES DEPARTMENT OF COMMERCE

United States Patent and Trademark Office

May 04, 2000

09/914451

THIS IS TO CERTIFY THAT ANNEXED HERETO IS A TRUE COPY FROM THE RECORDS OF THE UNITED STATES PATENT AND TRADEMARK OFFICE OF THOSE PAPERS OF THE BELOW IDENTIFIED PATENT APPLICATION THAT MET THE REQUIREMENTS TO BE GRANTED A FILING DATE UNDER 35 USC 111.

APPLICATION NUMBER: 60/122,110


FILING DATE: February 26, 1999

## PRIORITY DOCUMENT

SUBMITTED OR TRANSMITTED IN  
COMPLIANCE WITH RULE 17.1(a) OR (b)



By Authority of the  
COMMISSIONER OF PATENTS AND TRADEMARKS

  
P. SWAIN  
Certifying Officer

PART (2) OF (2) PART(S)



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 1290 | O   | VAL | A | 167 | 9.902  | 56.532 | 47.879 | 1.00 | 40.91 |
| ATOM | 1291 | CB  | VAL | A | 167 | 12.549 | 56.860 | 46.048 | 1.00 | 31.28 |
| ATOM | 1292 | CG1 | VAL | A | 167 | 12.854 | 55.542 | 45.329 | 1.00 | 28.20 |
| ATOM | 1293 | CG2 | VAL | A | 167 | 13.456 | 57.964 | 45.565 | 1.00 | 31.06 |
| ATOM | 1294 | N   | ALA | A | 168 | 10.217 | 55.019 | 46.257 | 1.00 | 36.46 |
| ATOM | 1295 | CA  | ALA | A | 168 | 9.584  | 53.935 | 46.979 | 1.00 | 35.14 |
| ATOM | 1296 | C   | ALA | A | 168 | 10.418 | 52.662 | 46.836 | 1.00 | 43.27 |
| ATOM | 1297 | O   | ALA | A | 168 | 10.889 | 52.343 | 45.733 | 1.00 | 44.74 |
| ATOM | 1298 | CB  | ALA | A | 168 | 8.149  | 53.700 | 46.550 | 1.00 | 34.20 |
| ATOM | 1299 | N   | LEU | A | 169 | 10.603 | 51.960 | 47.975 | 1.00 | 35.27 |
| ATOM | 1300 | CA  | LEU | A | 169 | 11.323 | 50.696 | 48.069 | 1.00 | 29.39 |
| ATOM | 1301 | C   | LEU | A | 169 | 10.491 | 49.635 | 48.797 | 1.00 | 33.87 |
| ATOM | 1302 | O   | LEU | A | 169 | 9.604  | 49.918 | 49.613 | 1.00 | 31.21 |
| ATOM | 1303 | CB  | LEU | A | 169 | 12.721 | 50.835 | 48.656 | 1.00 | 28.62 |
| ATOM | 1304 | CG  | LEU | A | 169 | 13.593 | 51.810 | 47.891 | 1.00 | 35.90 |
| ATOM | 1305 | CD1 | LEU | A | 169 | 14.953 | 51.819 | 48.558 | 1.00 | 39.38 |
| ATOM | 1306 | CD2 | LEU | A | 169 | 13.765 | 51.394 | 46.432 | 1.00 | 37.35 |
| ATOM | 1307 | N   | MET | A | 170 | 10.758 | 48.381 | 48.479 | 1.00 | 34.23 |
| ATOM | 1308 | CA  | MET | A | 170 | 10.012 | 47.291 | 49.069 | 1.00 | 31.07 |
| ATOM | 1309 | C   | MET | A | 170 | 10.874 | 46.083 | 49.287 | 1.00 | 34.13 |
| ATOM | 1310 | O   | MET | A | 170 | 11.995 | 45.973 | 48.775 | 1.00 | 35.20 |
| ATOM | 1311 | CB  | MET | A | 170 | 8.842  | 46.882 | 48.154 | 1.00 | 31.95 |
| ATOM | 1312 | CG  | MET | A | 170 | 7.751  | 47.934 | 48.116 | 1.00 | 33.13 |
| ATOM | 1313 | SD  | MET | A | 170 | 6.105  | 47.253 | 47.815 | 1.00 | 34.54 |
| ATOM | 1314 | CE  | MET | A | 170 | 5.820  | 46.349 | 49.363 | 1.00 | 32.25 |
| ATOM | 1315 | N   | SER | A | 171 | 10.332 | 45.165 | 50.057 | 1.00 | 28.20 |
| ATOM | 1316 | CA  | SER | A | 171 | 11.064 | 43.953 | 50.297 | 1.00 | 28.47 |
| ATOM | 1317 | C   | SER | A | 171 | 10.929 | 43.054 | 49.049 | 1.00 | 32.01 |
| ATOM | 1318 | O   | SER | A | 171 | 10.396 | 41.958 | 49.089 | 1.00 | 30.93 |
| ATOM | 1319 | CB  | SER | A | 171 | 10.662 | 43.265 | 51.606 | 1.00 | 30.93 |
| ATOM | 1320 | OG  | SER | A | 171 | 9.297  | 42.920 | 51.581 | 1.00 | 32.90 |
| ATOM | 1321 | N   | ALA | A | 172 | 11.401 | 43.543 | 47.912 | 1.00 | 28.84 |
| ATOM | 1322 | CA  | ALA | A | 172 | 11.286 | 42.773 | 46.691 | 1.00 | 29.48 |
| ATOM | 1323 | C   | ALA | A | 172 | 12.241 | 43.258 | 45.644 | 1.00 | 37.63 |
| ATOM | 1324 | O   | ALA | A | 172 | 13.060 | 44.147 | 45.881 | 1.00 | 35.07 |
| ATOM | 1325 | CB  | ALA | A | 172 | 9.884  | 42.969 | 46.120 | 1.00 | 29.48 |
| ATOM | 1326 | N   | ILE | A | 173 | 12.104 | 42.686 | 44.452 | 1.00 | 39.49 |
| ATOM | 1327 | CA  | ILE | A | 173 | 12.966 | 43.120 | 43.382 | 1.00 | 38.64 |
| ATOM | 1328 | C   | ILE | A | 173 | 12.418 | 44.343 | 42.648 | 1.00 | 44.83 |
| ATOM | 1329 | O   | ILE | A | 173 | 11.269 | 44.394 | 42.193 | 1.00 | 40.97 |
| ATOM | 1330 | CB  | ILE | A | 173 | 13.549 | 42.027 | 42.479 | 1.00 | 38.79 |
| ATOM | 1331 | CG1 | ILE | A | 173 | 14.258 | 40.970 | 43.302 | 1.00 | 37.40 |
| ATOM | 1332 | CG2 | ILE | A | 173 | 14.606 | 42.621 | 41.570 |      |       |



|      |      |     |     |   |     |        |        |        |      |        |
|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
| ATOM | 1351 | OD1 | ASP | A | 175 | 10.034 | 44.118 | 36.851 | 1.00 | 83.53  |
| ATOM | 1352 | OD2 | ASP | A | 175 | 7.910  | 44.176 | 37.558 | 1.00 | 92.45  |
| ATOM | 1353 | N   | GLY | A | 176 | 11.062 | 48.356 | 38.331 | 1.00 | 58.24  |
| ATOM | 1354 | CA  | GLY | A | 176 | 11.021 | 49.498 | 37.438 | 1.00 | 57.71  |
| ATOM | 1355 | C   | GLY | A | 176 | 9.969  | 50.546 | 37.773 | 1.00 | 58.98  |
| ATOM | 1356 | O   | GLY | A | 176 | 9.090  | 50.371 | 38.620 | 1.00 | 52.04  |
| ATOM | 1357 | N   | GLU | A | 177 | 10.110 | 51.649 | 37.050 | 1.00 | 63.72  |
| ATOM | 1358 | CA  | GLU | A | 177 | 9.267  | 52.812 | 37.172 | 1.00 | 67.79  |
| ATOM | 1359 | C   | GLU | A | 177 | 8.874  | 53.388 | 35.817 | 1.00 | 86.22  |
| ATOM | 1360 | O   | GLU | A | 177 | 9.614  | 53.364 | 34.830 | 1.00 | 91.14  |
| ATOM | 1361 | CB  | GLU | A | 177 | 9.986  | 53.902 | 38.006 | 1.00 | 68.25  |
| ATOM | 1362 | CG  | GLU | A | 177 | 11.432 | 54.145 | 37.519 | 1.00 | 71.58  |
| ATOM | 1363 | CD  | GLU | A | 177 | 12.183 | 55.088 | 38.404 | 1.00 | 85.08  |
| ATOM | 1364 | OE1 | GLU | A | 177 | 13.045 | 54.733 | 39.198 | 1.00 | 100.00 |
| ATOM | 1365 | OE2 | GLU | A | 177 | 11.765 | 56.316 | 38.264 | 1.00 | 56.71  |
| ATOM | 1366 | N   | THR | A | 178 | 7.671  | 53.924 | 35.835 | 1.00 | 84.76  |
| ATOM | 1367 | CA  | THR | A | 178 | 6.684  | 54.686 | 35.042 | 1.00 | 84.81  |
| ATOM | 1368 | C   | THR | A | 178 | 6.024  | 55.810 | 35.855 | 1.00 | 90.37  |
| ATOM | 1369 | O   | THR | A | 178 | 5.664  | 55.655 | 36.996 | 1.00 | 91.10  |
| ATOM | 1370 | CB  | THR | A | 178 | 5.618  | 53.713 | 34.561 | 1.00 | 89.82  |
| ATOM | 1371 | OG1 | THR | A | 178 | 5.283  | 52.830 | 35.636 | 1.00 | 80.25  |
| ATOM | 1372 | CG2 | THR | A | 178 | 6.161  | 52.898 | 33.396 | 1.00 | 93.46  |
| ATOM | 1373 | N   | PRO | A | 179 | 5.921  | 56.984 | 35.217 | 1.00 | 87.05  |
| ATOM | 1374 | CA  | PRO | A | 179 | 5.365  | 58.187 | 35.845 | 1.00 | 86.61  |
| ATOM | 1375 | C   | PRO | A | 179 | 3.857  | 58.419 | 35.531 | 1.00 | 89.04  |
| ATOM | 1376 | O   | PRO | A | 179 | 3.444  | 59.516 | 35.140 | 1.00 | 91.15  |
| ATOM | 1377 | CB  | PRO | A | 179 | 6.176  | 59.345 | 35.301 | 1.00 | 88.63  |
| ATOM | 1378 | CG  | PRO | A | 179 | 6.657  | 58.947 | 33.895 | 1.00 | 92.62  |
| ATOM | 1379 | CD  | PRO | A | 179 | 6.426  | 57.345 | 33.902 | 1.00 | 87.63  |
| ATOM | 1380 | N   | ASP | A | 180 | 3.020  | 57.347 | 35.694 | 1.00 | 82.31  |
| ATOM | 1381 | CA  | ASP | A | 180 | 1.616  | 57.568 | 35.310 | 1.00 | 81.19  |
| ATOM | 1382 | C   | ASP | A | 180 | 0.629  | 56.743 | 36.166 | 1.00 | 90.72  |
| ATOM | 1383 | O   | ASP | A | 180 | 0.533  | 55.519 | 36.072 | 1.00 | 91.13  |
| ATOM | 1384 | CB  | ASP | A | 180 | 1.458  | 57.196 | 33.827 | 1.00 | 82.12  |
| ATOM | 1385 | CG  | ASP | A | 180 | 0.087  | 57.651 | 33.327 | 1.00 | 95.94  |
| ATOM | 1386 | OD1 | ASP | A | 180 | -0.155 | 58.858 | 33.337 | 1.00 | 100.00 |
| ATOM | 1387 | OD2 | ASP | A | 180 | -0.714 | 56.801 | 32.946 | 1.00 | 94.36  |
| ATOM | 1388 | N   | PRO | A | 181 | -0.060 | 57.456 | 37.086 | 1.00 | 92.45  |
| ATOM | 1389 | CA  | PRO | A | 181 | -1.212 | 56.934 | 37.795 | 1.00 | 92.02  |
| ATOM | 1390 | C   | PRO | A | 181 | -2.519 | 57.566 | 37.284 | 1.00 | 100.00 |
| ATOM | 1391 | O   | PRO | A | 181 | -2.605 | 58.114 | 36.192 | 1.00 | 100.00 |
| ATOM | 1392 | CB  | PRO | A | 181 | -1.014 | 57.340 | 39.210 | 1.00 | 92.48  |
| ATOM | 1393 | CG  | PRO | A | 181 | -0.362 | 58.734 | 39.152 | 1.00 | 98.3   |



|        |      |     |     |   |     |        |        |        |      |        |
|--------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
| ATOM   | 1412 | N   | PRO | A | 184 | -4.187 | 60.906 | 43.237 | 1.00 | 97.96  |
| ATOM   | 1413 | CA  | PRO | A | 184 | -3.311 | 61.985 | 43.738 | 1.00 | 97.92  |
| ATOM   | 1414 | C   | PRO | A | 184 | -1.865 | 61.528 | 44.071 | 1.00 | 97.89  |
| ATOM   | 1415 | O   | PRO | A | 184 | -1.348 | 61.748 | 45.159 | 1.00 | 100.00 |
| ATOM   | 1416 | CB  | PRO | A | 184 | -3.973 | 62.561 | 44.992 | 1.00 | 98.86  |
| ATOM   | 1417 | CG  | PRO | A | 184 | -5.262 | 61.777 | 45.284 | 1.00 | 100.00 |
| ATOM   | 1418 | CD  | PRO | A | 184 | -5.122 | 60.532 | 44.284 | 1.00 | 97.20  |
| ATOM   | 1419 | N   | SER | A | 185 | -1.249 | 60.840 | 43.071 | 1.00 | 82.40  |
| ATOM   | 1420 | CA  | SER | A | 185 | 0.196  | 60.496 | 43.086 | 1.00 | 75.26  |
| ATOM   | 1421 | C   | SER | A | 185 | 0.748  | 60.563 | 41.623 | 1.00 | 71.88  |
| ATOM   | 1422 | O   | SER | A | 185 | -0.006 | 60.525 | 40.670 | 1.00 | 77.97  |
| ATOM   | 1423 | CB  | SER | A | 185 | 0.337  | 59.068 | 43.636 | 1.00 | 73.41  |
| ATOM   | 1424 | OG  | SER | A | 185 | 0.672  | 59.109 | 45.027 | 1.00 | 63.60  |
| ATOM   | 1425 | N   | ARG | A | 186 | 2.107  | 60.704 | 41.461 | 1.00 | 57.89  |
| ATOM   | 1426 | CA  | ARG | A | 186 | 2.650  | 60.971 | 40.088 | 1.00 | 56.00  |
| ATOM   | 1427 | C   | ARG | A | 186 | 3.725  | 59.943 | 39.633 | 1.00 | 59.64  |
| ATOM   | 1428 | O   | ARG | A | 186 | 4.473  | 60.157 | 38.688 | 1.00 | 60.30  |
| ATOM   | 1429 | CB  | ARG | A | 186 | 3.258  | 62.393 | 40.064 | 1.00 | 63.74  |
| ATOM   | 1430 | CG  | ARG | A | 186 | 2.339  | 63.457 | 40.677 | 1.00 | 80.44  |
| ATOM   | 1431 | CD  | ARG | A | 186 | 1.188  | 63.874 | 39.736 | 1.00 | 71.31  |
| ATOM   | 1432 | NE  | ARG | A | 186 | 1.316  | 63.215 | 38.436 | 1.00 | 79.64  |
| ATOM   | 1433 | CZ  | ARG | A | 186 | 0.185  | 62.862 | 37.784 | 1.00 | 95.30  |
| ATOM   | 1434 | NH1 | ARG | A | 186 | -0.999 | 63.109 | 38.312 | 1.00 | 56.25  |
| ATOM   | 1435 | NH2 | ARG | A | 186 | 0.276  | 62.232 | 36.603 | 1.00 | 89.98  |
| ATOM   | 1436 | N   | LYS | A | 187 | 3.892  | 58.778 | 40.265 | 1.00 | 54.50  |
| ATOM   | 1437 | CA  | LYS | A | 187 | 4.891  | 57.805 | 39.851 | 1.00 | 51.93  |
| ATOM   | 1438 | C   | LYS | A | 187 | 4.506  | 56.436 | 40.276 | 1.00 | 52.96  |
| ATOM   | 1439 | O   | LYS | A | 187 | 3.971  | 56.236 | 41.368 | 1.00 | 53.58  |
| ATOM   | 1440 | CB  | LYS | A | 187 | 6.247  | 58.047 | 40.470 | 1.00 | 53.78  |
| ATOM   | 1441 | CG  | LYS | A | 187 | 7.427  | 57.714 | 39.574 | 1.00 | 43.05  |
| ATOM   | 1442 | CD  | LYS | A | 187 | 8.517  | 58.761 | 39.762 | 1.00 | 53.36  |
| ATOM   | 1443 | CE  | LYS | A | 187 | 9.870  | 58.468 | 39.146 | 1.00 | 39.68  |
| ATOM   | 1444 | NZ  | LYS | A | 187 | 10.795 | 59.601 | 39.341 | 1.00 | 40.19  |
| ATOM   | 1445 | N   | ILE | A | 188 | 4.819  | 55.502 | 39.403 | 1.00 | 46.36  |
| ATOM   | 1446 | CA  | ILE | A | 188 | 4.565  | 54.128 | 39.700 | 1.00 | 43.57  |
| ATOM   | 1447 | C   | ILE | A | 188 | 5.824  | 53.311 | 39.851 | 1.00 | 42.64  |
| ATOM   | 1448 | O   | ILE | A | 188 | 6.647  | 53.189 | 38.937 | 1.00 | 41.55  |
| ATOM   | 1449 | CB  | ILE | A | 188 | 3.579  | 53.425 | 38.826 | 1.00 | 45.64  |
| ATOM   | 1450 | CG1 | ILE | A | 188 | 2.193  | 54.021 | 39.047 | 1.00 | 45.82  |
| ATOM   | 1451 | CG2 | ILE | A | 188 | 3.590  | 51.969 | 39.273 | 1.00 | 43.43  |
| ATOM   | 1452 | CD1 | ILE | A | 188 | 1.448  | 53.505 | 40.276 | 1.00 | 62.08  |
| ATOM   | 1453 | N   | TYR | A | 189 | 5.950  | 52.757 | 41.042 | 1.00 | 35.58  |
| ATOM   | 1454 | CA  | TYR | A | 189 | 7.079  | 51.933 | 41.356 | 1.00 | 37.57  |
| ATOM</ |      |     |     |   |     |        |        |        |      |        |



|      |      |     |     |   |     |        |          |        |            |
|------|------|-----|-----|---|-----|--------|----------|--------|------------|
| ATOM | 1473 | NZ  | LYS | A | 190 | 4.299  | 46.930   | 35.329 | 1.00100.00 |
| ATOM | 1474 | N   | PHE | A | 191 | 7.539  | 46.264   | 41.812 | 1.00 35.01 |
| ATOM | 1475 | CA  | PHE | A | 191 | 8.276  | 45.304   | 42.592 | 1.00 31.57 |
| ATOM | 1476 | C   | PHE | A | 191 | 7.792  | 43.871   | 42.465 | 1.00 30.89 |
| ATOM | 1477 | O   | PHE | A | 191 | 6.603  | 43.584   | 42.377 | 1.00 25.06 |
| ATOM | 1478 | CB  | PHE | A | 191 | 8.217  | 45.734   | 44.080 | 1.00 32.11 |
| ATOM | 1479 | CG  | PHE | A | 191 | 8.570  | 47.190   | 44.372 | 1.00 29.24 |
| ATOM | 1480 | CD1 | PHE | A | 191 | 9.895  | 47.593   | 44.539 | 1.00 31.81 |
| ATOM | 1481 | CD2 | PHE | A | 191 | 7.565  | 48.147   | 44.508 | 1.00 30.17 |
| ATOM | 1482 | CE1 | PHE | A | 191 | 10.230 | 48.925   | 44.805 | 1.00 34.10 |
| ATOM | 1483 | CE2 | PHE | A | 191 | 7.866  | 49.483   | 44.776 | 1.00 33.69 |
| ATOM | 1484 | CZ  | PHE | A | 191 | 9.201  | 49.860   | 44.928 | 1.00 33.32 |
| ATOM | 1485 | N   | ILE | A | 192 | 8.764  | 42.961   | 42.505 | 1.00 35.75 |
| ATOM | 1486 | CA  | ILE | A | 192 | 8.525  | 41.520   | 42.415 | 1.00 37.02 |
| ATOM | 1487 | C   | ILE | A | 192 | 9.255  | 40.653   | 43.469 | 1.00 33.05 |
| ATOM | 1488 | O   | ILE | A | 192 | 10.489 | 40.672   | 43.593 | 1.00 30.73 |
| ATOM | 1489 | CB  | ILE | A | 192 | 8.850  | 40.970   | 41.025 | 1.00 42.45 |
| ATOM | 1490 | CG1 | ILE | A | 192 | 8.289  | 41.914   | 39.981 | 1.00 46.39 |
| ATOM | 1491 | CG2 | ILE | A | 192 | 8.251  | 39.567   | 40.859 | 1.00 44.02 |
| ATOM | 1492 | CD1 | ILE | A | 192 | 7.609  | 41.231   | 38.798 | 1.00 69.61 |
| ATOM | 1493 | N   | GLN | A | 193 | 8.459  | 39.864   | 44.195 | 1.00 27.51 |
| ATOM | 1494 | CA  | GLN | A | 193 | 8.954  | 38.908   | 45.177 | 1.00 32.05 |
| ATOM | 1495 | C   | GLN | A | 193 | 8.626  | 37.488   | 44.757 | 1.00 44.32 |
| ATOM | 1496 | O   | GLN | A | 193 | 7.583  | 36.926   | 45.120 | 1.00 43.11 |
| ATOM | 1497 | CB  | GLN | A | 193 | 8.502  | 39.100   | 46.638 | 1.00 33.44 |
| ATOM | 1498 | CG  | GLN | A | 193 | 9.285  | 38.203   | 47.632 | 1.00 22.34 |
| ATOM | 1499 | CD  | GLN | A | 193 | 10.824 | 38.337   | 47.636 | 1.00 48.52 |
| ATOM | 1500 | OE1 | GLN | A | 193 | 11.557 | 37.537   | 47.016 | 1.00 45.24 |
| ATOM | 1501 | NE2 | GLN | A | 193 | 11.326 | 39.330   | 48.373 | 1.00 24.82 |
| ATOM | 1502 | N   | LYS | A | 194 | 9.543  | 36.908   | 43.993 | 1.00 46.91 |
| ATOM | 1503 | CA  | LYS | A | 194 | 9.384  | 35.540   | 43.529 | 1.00 47.56 |
| ATOM | 1504 | C   | LYS | A | 194 | 9.456  | 34.524   | 44.666 | 1.00 49.56 |
| ATOM | 1505 | O   | LYS | A | 194 | 8.777  | 33.520   | 44.598 | 1.00 50.85 |
| ATOM | 1506 | CB  | LYS | A | 194 | 10.385 | 35.159   | 42.439 | 1.00 48.11 |
| ATOM | 1507 | CG  | LYS | A | 194 | 9.884  | 35.443   | 41.031 | 1.00 55.70 |
| ATOM | 1508 | CD  | LYS | A | 194 | 10.895 | 36.200   | 40.179 | 1.00 67.67 |
| ATOM | 1509 | CE  | LYS | A | 194 | 10.614 | 36.122   | 38.682 | 1.00 81.92 |
| ATOM | 1510 | NZ  | LYS | A | 194 | 11.284 | 37.185   | 37.910 | 1.00 88.34 |
| ATOM | 1511 | N   | VAL | A | 195 | 10.308 | 34.753   | 45.689 | 1.00 39.55 |
| ATOM | 1512 | CA  | VAL | A | 195 | 10.422 | 33.780   | 46.764 | 1.00 33.56 |
| ATOM | 1513 | C   | VAL | A | 195 | 9.261  | 33.862   | 47.698 | 1.00 35.67 |
| ATOM | 1514 | O   | VAL | A | 195 | 8.804  | 34.945   | 48.034 | 1.00 38.69 |
| ATOM | 1515 | CB  | VAL | A | 195 | 11.716 | 33.844   | 47.560 | 1.00 32.62 |
| ATOM | 1516 | CG1 | VAL | A | 195 | 11.849 | 32.539   | 48.310 | 1.00 32.40 |
| ATOM | 1517 | CG2 | VAL | A | 195 | 12.933 | 34.029</ |        |            |



50122110-022699

|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 1534 | CA  | PRO | A | 198 | 5.647  | 35.110 | 55.410 | 1.00 | 31.31 |
| ATOM | 1535 | C   | PRO | A | 198 | 5.299  | 36.583 | 55.308 | 1.00 | 28.27 |
| ATOM | 1536 | O   | PRO | A | 198 | 6.212  | 37.391 | 55.115 | 1.00 | 22.70 |
| ATOM | 1537 | CB  | PRO | A | 198 | 6.252  | 34.849 | 56.794 | 1.00 | 31.17 |
| ATOM | 1538 | CG  | PRO | A | 198 | 7.768  | 34.768 | 56.615 | 1.00 | 34.94 |
| ATOM | 1539 | CD  | PRO | A | 198 | 8.057  | 34.706 | 55.122 | 1.00 | 32.99 |
| ATOM | 1540 | N   | CYS | A | 199 | 4.011  | 36.939 | 55.405 | 1.00 | 27.60 |
| ATOM | 1541 | CA  | CYS | A | 199 | 3.555  | 38.360 | 55.289 | 1.00 | 27.66 |
| ATOM | 1542 | C   | CYS | A | 199 | 4.255  | 39.390 | 56.187 | 1.00 | 30.13 |
| ATOM | 1543 | O   | CYS | A | 199 | 4.294  | 40.596 | 55.895 | 1.00 | 29.50 |
| ATOM | 1544 | CB  | CYS | A | 199 | 2.025  | 38.534 | 55.242 | 1.00 | 27.18 |
| ATOM | 1545 | SG  | CYS | A | 199 | 1.232  | 38.279 | 56.841 | 1.00 | 30.85 |
| ATOM | 1546 | N   | TYR | A | 200 | 4.847  | 38.903 | 57.270 | 1.00 | 26.15 |
| ATOM | 1547 | CA  | TYR | A | 200 | 5.538  | 39.798 | 58.123 | 1.00 | 28.28 |
| ATOM | 1548 | C   | TYR | A | 200 | 6.760  | 40.395 | 57.483 | 1.00 | 32.29 |
| ATOM | 1549 | O   | TYR | A | 200 | 7.359  | 41.286 | 58.036 | 1.00 | 31.56 |
| ATOM | 1550 | CB  | TYR | A | 200 | 5.844  | 39.215 | 59.489 | 1.00 | 30.59 |
| ATOM | 1551 | CG  | TYR | A | 200 | 6.989  | 38.272 | 59.568 | 1.00 | 28.28 |
| ATOM | 1552 | CD1 | TYR | A | 200 | 8.288  | 38.733 | 59.689 | 1.00 | 29.48 |
| ATOM | 1553 | CD2 | TYR | A | 200 | 6.756  | 36.903 | 59.475 | 1.00 | 27.55 |
| ATOM | 1554 | CE1 | TYR | A | 200 | 9.377  | 37.862 | 59.825 | 1.00 | 21.42 |
| ATOM | 1555 | CE2 | TYR | A | 200 | 7.838  | 36.015 | 59.595 | 1.00 | 27.41 |
| ATOM | 1556 | CZ  | TYR | A | 200 | 9.144  | 36.488 | 59.737 | 1.00 | 25.11 |
| ATOM | 1557 | OH  | TYR | A | 200 | 10.215 | 35.614 | 59.880 | 1.00 | 27.62 |
| ATOM | 1558 | N   | LEU | A | 201 | 7.113  | 39.897 | 56.313 | 1.00 | 31.66 |
| ATOM | 1559 | CA  | LEU | A | 201 | 8.278  | 40.378 | 55.579 | 1.00 | 29.49 |
| ATOM | 1560 | C   | LEU | A | 201 | 7.914  | 41.343 | 54.484 | 1.00 | 33.65 |
| ATOM | 1561 | O   | LEU | A | 201 | 8.767  | 41.737 | 53.686 | 1.00 | 35.31 |
| ATOM | 1562 | CB  | LEU | A | 201 | 9.225  | 39.275 | 55.035 | 1.00 | 27.04 |
| ATOM | 1563 | CG  | LEU | A | 201 | 9.697  | 38.271 | 56.071 | 1.00 | 27.42 |
| ATOM | 1564 | CD1 | LEU | A | 201 | 10.254 | 37.030 | 55.390 | 1.00 | 23.71 |
| ATOM | 1565 | CD2 | LEU | A | 201 | 10.764 | 38.913 | 56.957 | 1.00 | 30.55 |
| ATOM | 1566 | N   | ILE | A | 202 | 6.648  | 41.710 | 54.438 | 1.00 | 28.66 |
| ATOM | 1567 | CA  | ILE | A | 202 | 6.249  | 42.674 | 53.433 | 1.00 | 29.57 |
| ATOM | 1568 | C   | ILE | A | 202 | 6.636  | 44.074 | 53.951 | 1.00 | 40.28 |
| ATOM | 1569 | O   | ILE | A | 202 | 6.192  | 44.493 | 55.027 | 1.00 | 40.75 |
| ATOM | 1570 | CB  | ILE | A | 202 | 4.733  | 42.651 | 53.182 | 1.00 | 31.18 |
| ATOM | 1571 | CG1 | ILE | A | 202 | 4.250  | 41.429 | 52.405 | 1.00 | 28.21 |
| ATOM | 1572 | CG2 | ILE | A | 202 | 4.259  | 43.962 | 52.521 | 1.00 | 29.23 |
| ATOM | 1573 | CD1 | ILE | A | 202 | 2.724  | 41.288 | 52.449 | 1.00 | 23.01 |
| ATOM | 1574 | N   | ALA | A | 203 | 7.445  | 44.813 | 53.197 | 1.00 | 39.14 |
| ATOM | 1575 | CA  | ALA | A | 203 | 7.840  | 46.150 | 53.611 | 1.00 | 37.03 |
| ATOM | 1576 | C   | ALA | A | 203 | 7.819  | 47.159 | 52.482 | 1.00 | 34.32 |
| ATOM | 1577 | O   | ALA | A | 203 | 8.060  | 46.836 | 51.311 | 1.00 | 30.63 |
| ATOM | 1578 | CB  | ALA | A | 203 | 9.180  | 46.143 | 54.309 | 1.00 | 38.22 |
| ATOM | 1579 | N   | LEU | A | 204 | 7.514  | 48.388 | 52.910 | 1.00 | 33.64 |
| ATOM | 1580 | CA  | LEU | A | 204 | 7.388  | 49.604 | 52.102 | 1.00 | 32.56 |
| ATOM | 1581 | C   | LEU | A | 204 | 7.993  | 50.817 | 52.812 | 1.00 | 37.69 |
| ATOM | 1582 | O   | LEU | A | 204 | 7.854  | 51.037 | 54.034 | 1.00 | 32.66 |
| ATOM | 1583 | CB  | LEU | A | 204 | 5.906  | 49.929 | 51.718 | 1.00 | 29.74 |
| ATOM | 1584 | CG  | LEU | A | 204 | 5.706  | 51.182 | 50.855 | 1.00 | 29.64 |
| ATOM | 1585 | CD1 | LEU | A | 204 | 6.263  | 50.994 | 49.445 | 1.00 | 29.47 |
| ATOM | 1586 | CD2 | LEU | A | 204 | 4.222  | 51.515 | 50.750 | 1.00 | 33.50 |
| ATOM | 1587 | N   | VAL | A | 205 | 8.670  | 51.603 | 51.991 | 1.00 | 36.87 |
| ATOM | 1588 | CA  | VAL | A | 205 | 9.305  | 52.821 | 52.415 | 1.00 | 35.15 |
| ATOM | 1589 | C   | VAL | A | 205 | 9.224  | 53.795 | 51.284 | 1.00 | 38.41 |
| ATOM | 1590 | O   | VAL | A | 205 | 9.575  | 53.462 | 50.148 | 1.00 | 39.50 |
| ATOM | 1591 | CB  | VAL | A | 205 | 10.769 | 52.651 | 52.804 | 1.00 | 36.06 |
| ATOM | 1592 | CG1 | VAL | A | 205 | 11.466 | 51.794 | 51.757 | 1.00 | 35.08 |
| ATOM | 1593 | CG2 | VAL | A | 205 | 11.432 | 54.020 | 52.833 | 1.00 | 35.98 |
| ATOM | 1594 | N   | VAL | A | 206 | 8.750  | 54.983 | 51.623 | 1.00 | 33.54 |



|      |      |     |     |   |     |        |        |        |      |        |
|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
| ATOM | 1595 | CA  | VAL | A | 206 | 8.623  | 56.104 | 50.687 | 1.00 | 31.81  |
| ATOM | 1596 | C   | VAL | A | 206 | 9.300  | 57.343 | 51.249 | 1.00 | 31.62  |
| ATOM | 1597 | O   | VAL | A | 206 | 9.076  | 57.722 | 52.406 | 1.00 | 34.81  |
| ATOM | 1598 | CB  | VAL | A | 206 | 7.179  | 56.405 | 50.305 | 1.00 | 33.35  |
| ATOM | 1599 | CG1 | VAL | A | 206 | 7.129  | 57.243 | 49.029 | 1.00 | 33.44  |
| ATOM | 1600 | CG2 | VAL | A | 206 | 6.452  | 55.084 | 50.109 | 1.00 | 31.98  |
| ATOM | 1601 | N   | GLY | A | 207 | 10.130 | 57.959 | 50.431 | 1.00 | 24.94  |
| ATOM | 1602 | CA  | GLY | A | 207 | 10.807 | 59.168 | 50.861 | 1.00 | 27.25  |
| ATOM | 1603 | C   | GLY | A | 207 | 11.802 | 59.632 | 49.838 | 1.00 | 38.81  |
| ATOM | 1604 | O   | GLY | A | 207 | 12.046 | 58.966 | 48.840 | 1.00 | 39.82  |
| ATOM | 1605 | N   | ALA | A | 208 | 12.375 | 60.783 | 50.113 | 1.00 | 41.07  |
| ATOM | 1606 | CA  | ALA | A | 208 | 13.370 | 61.354 | 49.233 | 1.00 | 42.72  |
| ATOM | 1607 | C   | ALA | A | 208 | 14.660 | 60.550 | 49.356 | 1.00 | 49.10  |
| ATOM | 1608 | O   | ALA | A | 208 | 15.651 | 60.997 | 49.957 | 1.00 | 51.30  |
| ATOM | 1609 | CB  | ALA | A | 208 | 13.605 | 62.810 | 49.589 | 1.00 | 42.95  |
| ATOM | 1610 | N   | LEU | A | 209 | 14.623 | 59.350 | 48.773 | 1.00 | 40.92  |
| ATOM | 1611 | CA  | LEU | A | 209 | 15.739 | 58.440 | 48.825 | 1.00 | 39.55  |
| ATOM | 1612 | C   | LEU | A | 209 | 16.756 | 58.575 | 47.743 | 1.00 | 47.96  |
| ATOM | 1613 | O   | LEU | A | 209 | 16.420 | 58.843 | 46.597 | 1.00 | 49.44  |
| ATOM | 1614 | CB  | LEU | A | 209 | 15.269 | 56.994 | 48.894 | 1.00 | 37.97  |
| ATOM | 1615 | CG  | LEU | A | 209 | 14.420 | 56.803 | 50.129 | 1.00 | 40.46  |
| ATOM | 1616 | CD1 | LEU | A | 209 | 13.713 | 55.469 | 50.075 | 1.00 | 36.99  |
| ATOM | 1617 | CD2 | LEU | A | 209 | 15.283 | 56.921 | 51.387 | 1.00 | 43.31  |
| ATOM | 1618 | N   | GLU | A | 210 | 17.999 | 58.317 | 48.182 | 1.00 | 42.68  |
| ATOM | 1619 | CA  | GLU | A | 210 | 19.205 | 58.311 | 47.381 | 1.00 | 40.30  |
| ATOM | 1620 | C   | GLU | A | 210 | 19.965 | 57.056 | 47.693 | 1.00 | 47.51  |
| ATOM | 1621 | O   | GLU | A | 210 | 19.708 | 56.432 | 48.721 | 1.00 | 47.89  |
| ATOM | 1622 | CB  | GLU | A | 210 | 20.084 | 59.553 | 47.613 | 1.00 | 42.01  |
| ATOM | 1623 | CG  | GLU | A | 210 | 19.699 | 60.734 | 46.697 | 1.00 | 58.26  |
| ATOM | 1624 | CD  | GLU | A | 210 | 20.524 | 61.970 | 46.897 | 1.00 | 100.00 |
| ATOM | 1625 | OE1 | GLU | A | 210 | 21.629 | 61.968 | 47.451 | 1.00 | 95.26  |
| ATOM | 1626 | OE2 | GLU | A | 210 | 19.935 | 63.047 | 46.486 | 1.00 | 100.00 |
| ATOM | 1627 | N   | SER | A | 211 | 20.895 | 56.662 | 46.805 | 1.00 | 45.01  |
| ATOM | 1628 | CA  | SER | A | 211 | 21.661 | 55.442 | 47.013 | 1.00 | 42.25  |
| ATOM | 1629 | C   | SER | A | 211 | 23.143 | 55.535 | 46.667 | 1.00 | 43.37  |
| ATOM | 1630 | O   | SER | A | 211 | 23.649 | 56.493 | 46.086 | 1.00 | 46.43  |
| ATOM | 1631 | CB  | SER | A | 211 | 21.025 | 54.233 | 46.346 | 1.00 | 44.33  |
| ATOM | 1632 | OG  | SER | A | 211 | 21.274 | 54.244 | 44.934 | 1.00 | 54.15  |
| ATOM | 1633 | N   | ARG | A | 212 | 23.829 | 54.497 | 47.053 | 1.00 | 34.85  |
| ATOM | 1634 | CA  | ARG | A | 212 | 25.229 | 54.328 | 46.791 | 1.00 | 35.41  |
| ATOM | 1635 | C   | ARG | A | 212 | 25.430 | 52.838 | 46.567 | 1.00 | 45.39  |
| ATOM | 1636 | O   | ARG | A | 212 | 24.840 | 52.027 | 47.276 | 1.00 | 48.85  |
| ATOM | 1637 | CB  | ARG | A | 212 | 26.101 | 54.846 | 47.915 | 1.00 | 37.25  |
| ATOM | 1638 | CG  | ARG | A | 212 | 27.151 | 55.827 | 47.402 | 1.00 | 68.10  |
| ATOM | 1639 | CD  | ARG | A | 212 | 26.532 | 56.962 | 46.587 | 1.00 | 76.55  |
| ATOM | 1640 | NE  | ARG | A | 212 | 26.695 | 58.307 | 47.148 | 1.00 | 55.19  |
| ATOM | 1641 | CZ  | ARG | A | 212 | 25.845 | 59.301 | 46.867 | 1.00 | 70.87  |
| ATOM | 1642 | NH1 | ARG | A | 212 | 24.806 | 59.105 | 46.059 | 1.00 | 35.71  |
| ATOM | 1643 | NH2 | ARG | A | 212 | 26.032 | 60.516 | 47.392 | 1.00 | 73.35  |
| ATOM | 1644 | N   | GLN | A | 213 | 26.210 | 52.442 | 45.567 | 1.00 | 40.74  |
| ATOM | 1645 | CA  | GLN | A | 213 | 26.408 | 51.021 | 45.331 | 1.00 | 39.90  |
| ATOM | 1646 | C   | GLN | A | 213 | 27.646 | 50.537 | 46.050 | 1.00 | 46.34  |
| ATOM | 1647 | O   | GLN | A | 213 | 28.740 | 50.981 | 45.741 | 1.00 | 53.77  |
| ATOM | 1648 | CB  | GLN | A | 213 | 26.545 | 50.741 | 43.846 | 1.00 | 40.99  |
| ATOM | 1649 | CG  | GLN | A | 213 | 26.976 | 49.296 | 43.532 | 1.00 | 55.79  |
| ATOM | 1650 | CD  | GLN | A | 213 | 26.292 | 48.743 | 42.301 | 1.00 | 76.04  |
| ATOM | 1651 | OE1 | GLN | A | 213 | 26.275 | 47.523 | 42.102 | 1.00 | 86.66  |
| ATOM | 1652 | NE2 | GLN | A | 213 | 25.700 | 49.618 | 41.489 | 1.00 | 55.45  |
| ATOM | 1653 | N   | ILE | A | 214 | 27.495 | 49.649 | 47.013 | 1.00 | 33.12  |
| ATOM | 1654 | CA  | ILE | A | 214 | 28.663 | 49.206 | 47.743 | 1.00 | 32.55  |
| ATOM | 1655 | C   | ILE | A | 214 | 28.911 | 47.765 | 47.536 | 1.00 | 39.29  |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 1656 | O   | ILE | A | 214 | 29.726 | 47.162 | 48.230 | 1.00 | 42.41 |
| ATOM | 1657 | CB  | ILE | A | 214 | 28.546 | 49.428 | 49.250 | 1.00 | 35.72 |
| ATOM | 1658 | CG1 | ILE | A | 214 | 27.395 | 48.573 | 49.791 | 1.00 | 36.13 |
| ATOM | 1659 | CG2 | ILE | A | 214 | 28.344 | 50.911 | 49.598 | 1.00 | 35.79 |
| ATOM | 1660 | CD1 | ILE | A | 214 | 27.067 | 48.841 | 51.260 | 1.00 | 46.69 |
| ATOM | 1661 | N   | GLY | A | 215 | 28.199 | 47.197 | 46.598 | 1.00 | 35.02 |
| ATOM | 1662 | CA  | GLY | A | 215 | 28.638 | 45.855 | 46.234 | 1.00 | 34.88 |
| ATOM | 1663 | C   | GLY | A | 215 | 27.970 | 45.405 | 44.950 | 1.00 | 41.09 |
| ATOM | 1664 | O   | GLY | A | 215 | 27.083 | 46.048 | 44.425 | 1.00 | 44.25 |
| ATOM | 1665 | N   | PRO | A | 216 | 28.448 | 44.262 | 44.410 | 1.00 | 39.62 |
| ATOM | 1666 | CA  | PRO | A | 216 | 27.890 | 43.720 | 43.197 | 1.00 | 39.66 |
| ATOM | 1667 | C   | PRO | A | 216 | 26.369 | 43.661 | 43.253 | 1.00 | 41.56 |
| ATOM | 1668 | O   | PRO | A | 216 | 25.655 | 43.817 | 42.240 | 1.00 | 44.35 |
| ATOM | 1669 | CB  | PRO | A | 216 | 28.448 | 42.311 | 42.996 | 1.00 | 39.91 |
| ATOM | 1670 | CG  | PRO | A | 216 | 29.377 | 41.993 | 44.164 | 1.00 | 41.54 |
| ATOM | 1671 | CD  | PRO | A | 216 | 29.514 | 43.411 | 44.897 | 1.00 | 37.70 |
| ATOM | 1672 | N   | ARG | A | 217 | 25.846 | 43.398 | 44.477 | 1.00 | 31.04 |
| ATOM | 1673 | CA  | ARG | A | 217 | 24.421 | 43.328 | 44.652 | 1.00 | 29.22 |
| ATOM | 1674 | C   | ARG | A | 217 | 23.928 | 44.109 | 45.872 | 1.00 | 38.24 |
| ATOM | 1675 | O   | ARG | A | 217 | 22.861 | 43.885 | 46.368 | 1.00 | 40.69 |
| ATOM | 1676 | CB  | ARG | A | 217 | 24.012 | 41.844 | 44.790 | 1.00 | 22.75 |
| ATOM | 1677 | CG  | ARG | A | 217 | 25.221 | 40.963 | 45.109 | 1.00 | 40.77 |
| ATOM | 1678 | CD  | ARG | A | 217 | 24.828 | 39.774 | 45.985 | 1.00 | 34.08 |
| ATOM | 1679 | NE  | ARG | A | 217 | 26.020 | 39.183 | 46.581 | 1.00 | 45.20 |
| ATOM | 1680 | CZ  | ARG | A | 217 | 25.955 | 37.894 | 46.911 | 1.00 | 65.13 |
| ATOM | 1681 | NH1 | ARG | A | 217 | 24.832 | 37.220 | 46.716 | 1.00 | 42.40 |
| ATOM | 1682 | NH2 | ARG | A | 217 | 26.997 | 37.300 | 47.472 | 1.00 | 48.08 |
| ATOM | 1683 | N   | THR | A | 218 | 24.784 | 45.022 | 46.404 | 1.00 | 31.00 |
| ATOM | 1684 | CA  | THR | A | 218 | 24.309 | 45.886 | 47.487 | 1.00 | 31.00 |
| ATOM | 1685 | C   | THR | A | 218 | 24.128 | 47.319 | 47.021 | 1.00 | 43.60 |
| ATOM | 1686 | O   | THR | A | 218 | 25.065 | 47.930 | 46.512 | 1.00 | 48.42 |
| ATOM | 1687 | CB  | THR | A | 218 | 25.315 | 45.845 | 48.640 | 1.00 | 36.95 |
| ATOM | 1688 | OG1 | THR | A | 218 | 25.430 | 44.517 | 49.139 | 1.00 | 45.66 |
| ATOM | 1689 | CG2 | THR | A | 218 | 24.826 | 46.751 | 49.766 | 1.00 | 34.17 |
| ATOM | 1690 | N   | LEU | A | 219 | 23.099 | 48.018 | 47.431 | 1.00 | 39.19 |
| ATOM | 1691 | CA  | LEU | A | 219 | 23.055 | 49.452 | 47.315 | 1.00 | 38.18 |
| ATOM | 1692 | C   | LEU | A | 219 | 22.713 | 50.000 | 48.695 | 1.00 | 42.32 |
| ATOM | 1693 | O   | LEU | A | 219 | 22.108 | 49.289 | 49.498 | 1.00 | 43.67 |
| ATOM | 1694 | CB  | LEU | A | 219 | 21.927 | 49.841 | 46.356 | 1.00 | 37.05 |
| ATOM | 1695 | CG  | LEU | A | 219 | 22.386 | 50.657 | 45.168 | 1.00 | 39.31 |
| ATOM | 1696 | CD1 | LEU | A | 219 | 23.670 | 50.064 | 44.613 | 1.00 | 40.57 |
| ATOM | 1697 | CD2 | LEU | A | 219 | 21.283 | 50.619 | 44.131 | 1.00 | 29.39 |
| ATOM | 1698 | N   | VAL | A | 220 | 23.066 | 51.    |        |      |       |



|      |      |     |     |   |     |        |        |        |      |        |
|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
| ATOM | 1717 | CZ3 | TRP | A | 221 | 17.054 | 54.083 | 45.710 | 1.00 | 39.08  |
| ATOM | 1718 | CH2 | TRP | A | 221 | 17.360 | 53.040 | 44.864 | 1.00 | 38.48  |
| ATOM | 1719 | N   | SER | A | 222 | 19.271 | 55.896 | 51.688 | 1.00 | 37.01  |
| ATOM | 1720 | CA  | SER | A | 222 | 19.017 | 56.846 | 52.748 | 1.00 | 38.05  |
| ATOM | 1721 | C   | SER | A | 222 | 18.853 | 58.251 | 52.205 | 1.00 | 45.28  |
| ATOM | 1722 | O   | SER | A | 222 | 19.005 | 58.503 | 51.008 | 1.00 | 44.02  |
| ATOM | 1723 | CB  | SER | A | 222 | 20.098 | 56.816 | 53.820 | 1.00 | 39.07  |
| ATOM | 1724 | OG  | SER | A | 222 | 21.322 | 57.149 | 53.229 | 1.00 | 42.36  |
| ATOM | 1725 | N   | GLU | A | 223 | 18.586 | 59.190 | 53.088 | 1.00 | 40.91  |
| ATOM | 1726 | CA  | GLU | A | 223 | 18.465 | 60.527 | 52.584 | 1.00 | 41.97  |
| ATOM | 1727 | C   | GLU | A | 223 | 19.843 | 61.042 | 52.234 | 1.00 | 50.17  |
| ATOM | 1728 | O   | GLU | A | 223 | 20.829 | 60.701 | 52.863 | 1.00 | 52.02  |
| ATOM | 1729 | CB  | GLU | A | 223 | 17.856 | 61.483 | 53.597 | 1.00 | 43.06  |
| ATOM | 1730 | CG  | GLU | A | 223 | 16.364 | 61.262 | 53.861 | 1.00 | 51.71  |
| ATOM | 1731 | CD  | GLU | A | 223 | 15.799 | 62.478 | 54.545 | 1.00 | 84.51  |
| ATOM | 1732 | OE1 | GLU | A | 223 | 15.905 | 63.610 | 54.085 | 1.00 | 56.82  |
| ATOM | 1733 | OE2 | GLU | A | 223 | 15.244 | 62.222 | 55.705 | 1.00 | 88.87  |
| ATOM | 1734 | N   | LYS | A | 224 | 19.892 | 61.875 | 51.229 | 1.00 | 47.39  |
| ATOM | 1735 | CA  | LYS | A | 224 | 21.139 | 62.456 | 50.792 | 1.00 | 48.51  |
| ATOM | 1736 | C   | LYS | A | 224 | 22.163 | 62.683 | 51.930 | 1.00 | 50.90  |
| ATOM | 1737 | O   | LYS | A | 224 | 23.382 | 62.569 | 51.736 | 1.00 | 51.55  |
| ATOM | 1738 | CB  | LYS | A | 224 | 20.843 | 63.736 | 49.986 | 1.00 | 51.58  |
| ATOM | 1739 | CG  | LYS | A | 224 | 22.039 | 64.648 | 49.723 | 1.00 | 81.16  |
| ATOM | 1740 | CD  | LYS | A | 224 | 21.954 | 65.397 | 48.392 | 1.00 | 97.82  |
| ATOM | 1741 | CE  | LYS | A | 224 | 21.646 | 66.891 | 48.530 | 1.00 | 100.00 |
| ATOM | 1742 | NZ  | LYS | A | 224 | 22.056 | 67.700 | 47.362 | 1.00 | 100.00 |
| ATOM | 1743 | N   | GLU | A | 225 | 21.683 | 63.011 | 53.123 | 1.00 | 45.77  |
| ATOM | 1744 | CA  | GLU | A | 225 | 22.607 | 63.309 | 54.199 | 1.00 | 46.00  |
| ATOM | 1745 | C   | GLU | A | 225 | 23.227 | 62.150 | 54.902 | 1.00 | 47.99  |
| ATOM | 1746 | O   | GLU | A | 225 | 24.107 | 62.354 | 55.732 | 1.00 | 47.21  |
| ATOM | 1747 | CB  | GLU | A | 225 | 22.057 | 64.296 | 55.210 | 1.00 | 47.71  |
| ATOM | 1748 | CG  | GLU | A | 225 | 20.530 | 64.296 | 55.182 | 1.00 | 63.24  |
| ATOM | 1749 | CD  | GLU | A | 225 | 19.931 | 65.219 | 54.150 | 1.00 | 75.13  |
| ATOM | 1750 | OE1 | GLU | A | 225 | 20.187 | 66.420 | 54.046 | 1.00 | 54.64  |
| ATOM | 1751 | OE2 | GLU | A | 225 | 19.039 | 64.578 | 53.420 | 1.00 | 49.64  |
| ATOM | 1752 | N   | GLN | A | 226 | 22.798 | 60.949 | 54.564 | 1.00 | 43.92  |
| ATOM | 1753 | CA  | GLN | A | 226 | 23.340 | 59.772 | 55.224 | 1.00 | 43.91  |
| ATOM | 1754 | C   | GLN | A | 226 | 24.036 | 58.756 | 54.322 | 1.00 | 45.86  |
| ATOM | 1755 | O   | GLN | A | 226 | 24.756 | 57.871 | 54.806 | 1.00 | 45.70  |
| ATOM | 1756 | CB  | GLN | A | 226 | 22.252 | 59.084 | 56.063 | 1.00 | 45.27  |
| ATOM | 1757 | CG  | GLN | A | 226 | 21.965 | 59.790 | 57.400 | 1.00 | 31.17  |
| ATOM | 1758 | CD  | GLN | A | 226 | 21.297 | 61.155 | 57.302 | 1.00 | 44.48  |
| ATOM | 1759 | OE1 | GLN | A | 226 | 21.823 | 62.149 | 57.820 | 1.00 | 37.36  |
| ATOM | 1760 | NE2 | GLN | A | 226 | 20.115 | 61.202 | 56.696 | 1.00 | 30.28  |
| ATOM | 1761 | N   | VAL | A | 227 | 23.814 | 58.871 | 53.021 | 1.00 | 41.20  |
| ATOM | 1762 | CA  | VAL | A | 227 | 24.406 | 57.947 | 52.071 | 1.00 | 43.13  |
| ATOM | 1763 | C   | VAL | A | 227 | 25.884 | 57.670 | 52.261 | 1.00 | 50.55  |
| ATOM | 1764 | O   | VAL | A | 227 | 26.298 | 56.518 | 52.480 | 1.00 | 53.01  |
| ATOM | 1765 | CB  | VAL | A | 227 | 24.155 | 58.293 | 50.604 | 1.00 | 49.39  |
| ATOM | 1766 | CG1 | VAL | A | 227 | 24.319 | 57.029 | 49.771 | 1.00 | 48.89  |
| ATOM | 1767 | CG2 | VAL | A | 227 | 22.752 | 58.851 | 50.421 | 1.00 | 50.47  |
| ATOM | 1768 | N   | GLU | A | 228 | 26.696 | 58.718 | 52.170 | 1.00 | 44.08  |
| ATOM | 1769 | CA  | GLU | A | 228 | 28.123 | 58.542 | 52.310 | 1.00 | 41.71  |
| ATOM | 1770 | C   | GLU | A | 228 | 28.514 | 57.871 | 53.583 | 1.00 | 44.20  |
| ATOM | 1771 | O   | GLU | A | 228 | 29.227 | 56.868 | 53.589 | 1.00 | 44.88  |
| ATOM | 1772 | CB  | GLU | A | 228 | 28.935 | 59.824 | 52.102 | 1.00 | 43.08  |
| ATOM | 1773 | CG  | GLU | A | 228 | 29.153 | 60.161 | 50.611 | 1.00 | 64.74  |
| ATOM | 1774 | CD  | GLU | A | 228 | 29.114 | 58.965 | 49.701 | 1.00 | 84.29  |
| ATOM | 1775 | OE1 | GLU | A | 228 | 29.975 | 58.107 | 49.685 | 1.00 | 84.36  |
| ATOM | 1776 | OE2 | GLU | A | 228 | 28.064 | 58.951 | 48.917 | 1.00 | 73.81  |
| ATOM | 1777 | N   | LYS | A | 229 | 28.066 | 58.423 | 54.685 | 1.00 | 39.79  |



|      |      |     |     |   |     |        |        |        |      |        |
|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
| ATOM | 1778 | CA  | LYS | A | 229 | 28.449 | 57.796 | 55.922 | 1.00 | 39.04  |
| ATOM | 1779 | C   | LYS | A | 229 | 27.949 | 56.375 | 55.930 | 1.00 | 40.38  |
| ATOM | 1780 | O   | LYS | A | 229 | 28.639 | 55.433 | 56.346 | 1.00 | 43.63  |
| ATOM | 1781 | CB  | LYS | A | 229 | 28.129 | 58.585 | 57.187 | 1.00 | 39.79  |
| ATOM | 1782 | CG  | LYS | A | 229 | 28.903 | 58.072 | 58.394 | 1.00 | 63.75  |
| ATOM | 1783 | CD  | LYS | A | 229 | 28.498 | 58.763 | 59.685 | 1.00 | 77.46  |
| ATOM | 1784 | CE  | LYS | A | 229 | 29.677 | 59.084 | 60.593 | 1.00 | 94.73  |
| ATOM | 1785 | NZ  | LYS | A | 229 | 30.344 | 60.353 | 60.256 | 1.00 | 100.00 |
| ATOM | 1786 | N   | SER | A | 230 | 26.741 | 56.220 | 55.428 | 1.00 | 28.48  |
| ATOM | 1787 | CA  | SER | A | 230 | 26.174 | 54.891 | 55.377 | 1.00 | 25.93  |
| ATOM | 1788 | C   | SER | A | 230 | 27.089 | 53.988 | 54.587 | 1.00 | 30.26  |
| ATOM | 1789 | O   | SER | A | 230 | 27.469 | 52.855 | 54.955 | 1.00 | 28.48  |
| ATOM | 1790 | CB  | SER | A | 230 | 24.824 | 54.927 | 54.694 | 1.00 | 30.08  |
| ATOM | 1791 | OG  | SER | A | 230 | 23.822 | 55.293 | 55.605 | 1.00 | 41.60  |
| ATOM | 1792 | N   | ALA | A | 231 | 27.436 | 54.536 | 53.459 | 1.00 | 31.13  |
| ATOM | 1793 | CA  | ALA | A | 231 | 28.288 | 53.820 | 52.593 | 1.00 | 36.66  |
| ATOM | 1794 | C   | ALA | A | 231 | 29.597 | 53.383 | 53.270 | 1.00 | 47.68  |
| ATOM | 1795 | O   | ALA | A | 231 | 30.003 | 52.238 | 53.103 | 1.00 | 54.59  |
| ATOM | 1796 | CB  | ALA | A | 231 | 28.406 | 54.518 | 51.257 | 1.00 | 38.49  |
| ATOM | 1797 | N   | TYR | A | 232 | 30.256 | 54.246 | 54.060 | 1.00 | 40.77  |
| ATOM | 1798 | CA  | TYR | A | 232 | 31.500 | 53.830 | 54.730 | 1.00 | 38.40  |
| ATOM | 1799 | C   | TYR | A | 232 | 31.265 | 52.721 | 55.753 | 1.00 | 39.70  |
| ATOM | 1800 | O   | TYR | A | 232 | 32.041 | 51.772 | 55.862 | 1.00 | 36.46  |
| ATOM | 1801 | CB  | TYR | A | 232 | 32.311 | 54.981 | 55.414 | 1.00 | 38.27  |
| ATOM | 1802 | CG  | TYR | A | 232 | 33.497 | 54.525 | 56.303 | 1.00 | 42.36  |
| ATOM | 1803 | CD1 | TYR | A | 232 | 34.755 | 54.238 | 55.753 | 1.00 | 46.41  |
| ATOM | 1804 | CD2 | TYR | A | 232 | 33.373 | 54.394 | 57.691 | 1.00 | 40.99  |
| ATOM | 1805 | CE1 | TYR | A | 232 | 35.835 | 53.815 | 56.534 | 1.00 | 47.23  |
| ATOM | 1806 | CE2 | TYR | A | 232 | 34.441 | 53.979 | 58.496 | 1.00 | 40.10  |
| ATOM | 1807 | CZ  | TYR | A | 232 | 35.680 | 53.695 | 57.916 | 1.00 | 48.59  |
| ATOM | 1808 | OH  | TYR | A | 232 | 36.734 | 53.282 | 58.698 | 1.00 | 51.92  |
| ATOM | 1809 | N   | GLU | A | 233 | 30.191 | 52.883 | 56.519 | 1.00 | 35.75  |
| ATOM | 1810 | CA  | GLU | A | 233 | 29.835 | 51.984 | 57.606 | 1.00 | 34.55  |
| ATOM | 1811 | C   | GLU | A | 233 | 29.633 | 50.498 | 57.252 | 1.00 | 38.39  |
| ATOM | 1812 | O   | GLU | A | 233 | 30.152 | 49.576 | 57.892 | 1.00 | 38.55  |
| ATOM | 1813 | CB  | GLU | A | 233 | 28.673 | 52.623 | 58.414 | 1.00 | 34.48  |
| ATOM | 1814 | CG  | GLU | A | 233 | 28.666 | 52.262 | 59.912 | 1.00 | 24.95  |
| ATOM | 1815 | CD  | GLU | A | 233 | 29.463 | 53.183 | 60.787 | 1.00 | 37.55  |
| ATOM | 1816 | OE1 | GLU | A | 233 | 29.408 | 54.410 | 60.741 | 1.00 | 55.33  |
| ATOM | 1817 | OE2 | GLU | A | 233 | 30.216 | 52.518 | 61.619 | 1.00 | 40.65  |
| ATOM | 1818 | N   | PHE | A | 234 | 28.867 | 50.282 | 56.202 | 1.00 | 33.02  |
| ATOM | 1819 | CA  | PHE | A | 234 | 28.493 | 48.974 | 55.719 | 1.00 | 29.90  |
| ATOM | 1820 | C   | PHE | A | 234 | 29.341 | 48.398 | 54.592 | 1.00 | 34.69  |
| ATOM | 1821 | O   | PHE | A | 234 | 28.883 | 47.521 | 53.823 | 1.00 | 34.21  |
| ATOM | 1822 | CB  | PHE | A | 234 | 27.020 | 49.081 | 55.293 | 1.00 | 30.23  |
| ATOM | 1823 | CG  | PHE | A | 234 | 26.215 | 49.752 | 56.394 | 1.00 | 30.32  |
| ATOM | 1824 | CD1 | PHE | A | 234 | 26.518 | 49.521 | 57.739 | 1.00 | 31.50  |
| ATOM | 1825 | CD2 | PHE | A | 234 | 25.151 | 50.605 | 56.102 | 1.00 | 28.66  |
| ATOM | 1826 | CE1 | PHE | A | 234 | 25.780 | 50.103 | 58.772 | 1.00 | 30.43  |
| ATOM | 1827 | CE2 | PHE | A | 234 | 24.407 | 51.203 | 57.121 | 1.00 | 29.60  |
| ATOM | 1828 | CZ  | PHE | A | 234 | 24.725 | 50.959 | 58.458 | 1.00 | 27.47  |
| ATOM | 1829 | N   | SER | A | 235 | 30.571 | 48.874 | 54.476 | 1.00 | 29.55  |
| ATOM | 1830 | CA  | SER | A | 235 | 31.428 | 48.366 | 53.412 | 1.00 | 28.64  |
| ATOM | 1831 | C   | SER | A | 235 | 31.387 | 46.858 | 53.338 | 1.00 | 30.38  |
| ATOM | 1832 | O   | SER | A | 235 | 31.166 | 46.252 | 52.282 | 1.00 | 32.37  |
| ATOM | 1833 | CB  | SER | A | 235 | 32.861 | 48.787 | 53.604 | 1.00 | 31.15  |
| ATOM | 1834 | OG  | SER | A | 235 | 33.028 | 49.368 | 54.873 | 1.00 | 39.32  |
| ATOM | 1835 | N   | GLU | A | 236 | 31.698 | 46.299 | 54.504 | 1.00 | 22.49  |
| ATOM | 1836 | CA  | GLU | A | 236 | 31.815 | 44.873 | 54.737 | 1.00 | 23.79  |
| ATOM | 1837 | C   | GLU | A | 236 | 30.627 | 43.992 | 54.380 | 1.00 | 32.37  |
| ATOM | 1838 | O   | GLU | A | 236 | 30.697 | 42.772 | 54.545 | 1.00 | 29.91  |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 1839 | CB  | GLU | A | 236 | 32.305 | 44.529 | 56.134 | 1.00 | 24.06 |
| ATOM | 1840 | CG  | GLU | A | 236 | 33.491 | 45.403 | 56.585 | 1.00 | 22.96 |
| ATOM | 1841 | CD  | GLU | A | 236 | 33.600 | 45.492 | 58.090 | 1.00 | 66.18 |
| ATOM | 1842 | OE1 | GLU | A | 236 | 32.633 | 45.482 | 58.849 | 1.00 | 37.01 |
| ATOM | 1843 | OE2 | GLU | A | 236 | 34.848 | 45.518 | 58.494 | 1.00 | 78.68 |
| ATOM | 1844 | N   | THR | A | 237 | 29.560 | 44.593 | 53.891 | 1.00 | 34.11 |
| ATOM | 1845 | CA  | THR | A | 237 | 28.384 | 43.823 | 53.539 | 1.00 | 33.69 |
| ATOM | 1846 | C   | THR | A | 237 | 28.644 | 42.609 | 52.644 | 1.00 | 33.33 |
| ATOM | 1847 | O   | THR | A | 237 | 28.517 | 41.451 | 53.048 | 1.00 | 31.09 |
| ATOM | 1848 | CB  | THR | A | 237 | 27.218 | 44.710 | 53.057 | 1.00 | 37.99 |
| ATOM | 1849 | OG1 | THR | A | 237 | 26.899 | 45.675 | 54.048 | 1.00 | 33.49 |
| ATOM | 1850 | CG2 | THR | A | 237 | 25.995 | 43.862 | 52.744 | 1.00 | 25.66 |
| ATOM | 1851 | N   | GLU | A | 238 | 29.020 | 42.854 | 51.409 | 1.00 | 29.69 |
| ATOM | 1852 | CA  | GLU | A | 238 | 29.267 | 41.734 | 50.520 | 1.00 | 27.05 |
| ATOM | 1853 | C   | GLU | A | 238 | 30.071 | 40.638 | 51.146 | 1.00 | 33.17 |
| ATOM | 1854 | O   | GLU | A | 238 | 29.660 | 39.497 | 51.055 | 1.00 | 38.50 |
| ATOM | 1855 | CB  | GLU | A | 238 | 29.851 | 42.080 | 49.161 | 1.00 | 27.50 |
| ATOM | 1856 | CG  | GLU | A | 238 | 30.116 | 40.813 | 48.320 | 1.00 | 18.83 |
| ATOM | 1857 | CD  | GLU | A | 238 | 28.902 | 40.297 | 47.596 | 1.00 | 41.67 |
| ATOM | 1858 | OE1 | GLU | A | 238 | 27.848 | 40.909 | 47.464 | 1.00 | 33.59 |
| ATOM | 1859 | OE2 | GLU | A | 238 | 29.085 | 39.089 | 47.138 | 1.00 | 46.30 |
| ATOM | 1860 | N   | SER | A | 239 | 31.203 | 40.973 | 51.772 | 1.00 | 24.44 |
| ATOM | 1861 | CA  | SER | A | 239 | 32.045 | 39.957 | 52.387 | 1.00 | 24.60 |
| ATOM | 1862 | C   | SER | A | 239 | 31.245 | 39.060 | 53.344 | 1.00 | 35.72 |
| ATOM | 1863 | O   | SER | A | 239 | 31.379 | 37.830 | 53.360 | 1.00 | 35.25 |
| ATOM | 1864 | CB  | SER | A | 239 | 33.231 | 40.601 | 53.074 | 1.00 | 29.14 |
| ATOM | 1865 | OG  | SER | A | 239 | 32.747 | 41.590 | 53.961 | 1.00 | 54.60 |
| ATOM | 1866 | N   | MET | A | 240 | 30.382 | 39.703 | 54.154 | 1.00 | 33.13 |
| ATOM | 1867 | CA  | MET | A | 240 | 29.529 | 38.993 | 55.091 | 1.00 | 28.55 |
| ATOM | 1868 | C   | MET | A | 240 | 28.603 | 38.075 | 54.325 | 1.00 | 35.65 |
| ATOM | 1869 | O   | MET | A | 240 | 28.435 | 36.926 | 54.689 | 1.00 | 35.99 |
| ATOM | 1870 | CB  | MET | A | 240 | 28.736 | 39.945 | 55.993 | 1.00 | 26.50 |
| ATOM | 1871 | CG  | MET | A | 240 | 29.691 | 40.675 | 56.910 | 1.00 | 27.57 |
| ATOM | 1872 | SD  | MET | A | 240 | 28.871 | 41.986 | 57.833 | 1.00 | 32.91 |
| ATOM | 1873 | CE  | MET | A | 240 | 30.040 | 42.085 | 59.183 | 1.00 | 28.47 |
| ATOM | 1874 | N   | LEU | A | 241 | 28.019 | 38.603 | 53.243 | 1.00 | 32.77 |
| ATOM | 1875 | CA  | LEU | A | 241 | 27.120 | 37.859 | 52.381 | 1.00 | 29.87 |
| ATOM | 1876 | C   | LEU | A | 241 | 27.848 | 36.615 | 51.878 | 1.00 | 36.76 |
| ATOM | 1877 | O   | LEU | A | 241 | 27.302 | 35.509 | 51.858 | 1.00 | 36.97 |
| ATOM | 1878 | CB  | LEU | A | 241 | 26.715 | 38.753 | 51.196 | 1.00 | 29.71 |
| ATOM | 1879 | CG  | LEU | A | 241 | 25.283 | 39.289 | 51.237 | 1.00 | 37.68 |
| ATOM | 1880 | CD1 | LEU | A | 241 | 25.174 | 40.552 | 50.389 | 1.00 | 35.76 |
| ATOM | 1881 | CD2 | LEU | A | 241 | 24.    |        |        |      |       |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 1900 | CA  | ALA | A | 244 | 26.968 | 33.519 | 55.066 | 1.00 | 32.95 |
| ATOM | 1901 | C   | ALA | A | 244 | 26.600 | 32.392 | 54.127 | 1.00 | 36.35 |
| ATOM | 1902 | O   | ALA | A | 244 | 26.074 | 31.358 | 54.546 | 1.00 | 36.88 |
| ATOM | 1903 | CB  | ALA | A | 244 | 25.858 | 34.576 | 55.123 | 1.00 | 34.02 |
| ATOM | 1904 | N   | GLU | A | 245 | 26.890 | 32.617 | 52.846 | 1.00 | 31.20 |
| ATOM | 1905 | CA  | GLU | A | 245 | 26.614 | 31.635 | 51.818 | 1.00 | 29.26 |
| ATOM | 1906 | C   | GLU | A | 245 | 27.360 | 30.354 | 52.092 | 1.00 | 35.18 |
| ATOM | 1907 | O   | GLU | A | 245 | 26.849 | 29.276 | 51.800 | 1.00 | 36.21 |
| ATOM | 1908 | CB  | GLU | A | 245 | 26.908 | 32.177 | 50.421 | 1.00 | 30.22 |
| ATOM | 1909 | CG  | GLU | A | 245 | 25.701 | 32.938 | 49.842 | 1.00 | 39.79 |
| ATOM | 1910 | CD  | GLU | A | 245 | 26.026 | 33.564 | 48.529 | 1.00 | 51.91 |
| ATOM | 1911 | OE1 | GLU | A | 245 | 26.945 | 34.351 | 48.358 | 1.00 | 34.19 |
| ATOM | 1912 | OE2 | GLU | A | 245 | 25.246 | 33.142 | 47.585 | 1.00 | 47.48 |
| ATOM | 1913 | N   | ASP | A | 246 | 28.570 | 30.484 | 52.680 | 1.00 | 32.29 |
| ATOM | 1914 | CA  | ASP | A | 246 | 29.417 | 29.350 | 53.033 | 1.00 | 30.70 |
| ATOM | 1915 | C   | ASP | A | 246 | 28.848 | 28.645 | 54.230 | 1.00 | 35.47 |
| ATOM | 1916 | O   | ASP | A | 246 | 28.881 | 27.417 | 54.347 | 1.00 | 37.08 |
| ATOM | 1917 | CB  | ASP | A | 246 | 30.873 | 29.717 | 53.355 | 1.00 | 33.17 |
| ATOM | 1918 | CG  | ASP | A | 246 | 31.709 | 28.473 | 53.413 | 1.00 | 64.49 |
| ATOM | 1919 | OD1 | ASP | A | 246 | 31.934 | 27.789 | 52.437 | 1.00 | 67.15 |
| ATOM | 1920 | OD2 | ASP | A | 246 | 32.118 | 28.167 | 54.622 | 1.00 | 79.01 |
| ATOM | 1921 | N   | LEU | A | 247 | 28.323 | 29.434 | 55.134 | 1.00 | 33.59 |
| ATOM | 1922 | CA  | LEU | A | 247 | 27.731 | 28.868 | 56.334 | 1.00 | 36.70 |
| ATOM | 1923 | C   | LEU | A | 247 | 26.355 | 28.208 | 56.083 | 1.00 | 35.92 |
| ATOM | 1924 | O   | LEU | A | 247 | 26.060 | 27.110 | 56.551 | 1.00 | 30.77 |
| ATOM | 1925 | CB  | LEU | A | 247 | 27.562 | 29.954 | 57.435 | 1.00 | 38.34 |
| ATOM | 1926 | CG  | LEU | A | 247 | 28.732 | 30.100 | 58.394 | 1.00 | 44.30 |
| ATOM | 1927 | CD1 | LEU | A | 247 | 29.341 | 28.738 | 58.641 | 1.00 | 48.20 |
| ATOM | 1928 | CD2 | LEU | A | 247 | 29.779 | 31.013 | 57.815 | 1.00 | 35.25 |
| ATOM | 1929 | N   | GLY | A | 248 | 25.471 | 28.887 | 55.353 | 1.00 | 34.97 |
| ATOM | 1930 | CA  | GLY | A | 248 | 24.160 | 28.315 | 55.181 | 1.00 | 36.00 |
| ATOM | 1931 | C   | GLY | A | 248 | 23.754 | 27.976 | 53.778 | 1.00 | 37.99 |
| ATOM | 1932 | O   | GLY | A | 248 | 22.637 | 27.524 | 53.526 | 1.00 | 38.13 |
| ATOM | 1933 | N   | GLY | A | 249 | 24.637 | 28.158 | 52.849 | 1.00 | 30.74 |
| ATOM | 1934 | CA  | GLY | A | 249 | 24.203 | 27.852 | 51.526 | 1.00 | 30.15 |
| ATOM | 1935 | C   | GLY | A | 249 | 23.918 | 29.131 | 50.759 | 1.00 | 38.91 |
| ATOM | 1936 | O   | GLY | A | 249 | 24.126 | 30.240 | 51.238 | 1.00 | 41.32 |
| ATOM | 1937 | N   | PRO | A | 250 | 23.453 | 28.946 | 49.547 | 1.00 | 38.93 |
| ATOM | 1938 | CA  | PRO | A | 250 | 23.173 | 30.021 | 48.639 | 1.00 | 38.03 |
| ATOM | 1939 | C   | PRO | A | 250 | 22.203 | 31.078 | 49.096 | 1.00 | 42.17 |
| ATOM | 1940 | O   | PRO | A | 250 | 21.258 | 30.823 | 49.840 | 1.00 | 45.20 |
| ATOM | 1941 | CB  | PRO | A | 250 | 22.663 | 29.357 | 47.352 | 1.00 | 39.18 |
| ATOM | 1942 | CG  | PRO | A | 250 | 22.952 | 27.864 | 47.436 | 1.00 | 41.01 |
| ATOM | 1943 | CD  | PRO | A | 250 | 23.396 | 27.610 | 48.865 | 1.00 | 38.57 |
| ATOM | 1944 | N   | TYR | A | 251 | 22.486 | 32.275 | 48.600 | 1.00 | 35.37 |
| ATOM | 1945 | CA  | TYR | A | 251 | 21.692 | 33.461 | 48.817 | 1.00 | 34.87 |
| ATOM | 1946 | C   | TYR | A | 251 | 20.740 | 33.479 | 47.649 | 1.00 | 39.55 |
| ATOM | 1947 | O   | TYR | A | 251 | 21.125 | 33.794 | 46.535 | 1.00 | 42.57 |
| ATOM | 1948 | CB  | TYR | A | 251 | 22.540 | 34.759 | 48.790 | 1.00 | 35.07 |
| ATOM | 1949 | CG  | TYR | A | 251 | 21.711 | 35.980 | 49.119 | 1.00 | 35.25 |
| ATOM | 1950 | CD1 | TYR | A | 251 | 21.341 | 36.229 | 50.441 | 1.00 | 33.14 |
| ATOM | 1951 | CD2 | TYR | A | 251 | 21.260 | 36.846 | 48.121 | 1.00 | 37.98 |
| ATOM | 1952 | CE1 | TYR | A | 251 | 20.575 | 37.341 | 50.781 | 1.00 | 28.05 |
| ATOM | 1953 | CE2 | TYR | A | 251 | 20.492 | 37.967 | 48.443 | 1.00 | 40.05 |
| ATOM | 1954 | CZ  | TYR | A | 251 | 20.160 | 38.213 | 49.777 | 1.00 | 42.84 |
| ATOM | 1955 | OH  | TYR | A | 251 | 19.409 | 39.307 | 50.112 | 1.00 | 39.70 |
| ATOM | 1956 | N   | VAL | A | 252 | 19.510 | 33.102 | 47.914 | 1.00 | 32.21 |
| ATOM | 1957 | CA  | VAL | A | 252 | 18.495 | 33.003 | 46.899 | 1.00 | 30.05 |
| ATOM | 1958 | C   | VAL | A | 252 | 17.708 | 34.279 | 46.631 | 1.00 | 38.47 |
| ATOM | 1959 | O   | VAL | A | 252 | 17.000 | 34.340 | 45.640 | 1.00 | 40.65 |
| ATOM | 1960 | CB  | VAL | A | 252 | 17.560 | 31.845 | 47.253 | 1.00 | 31.27 |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 1961 | CG1 | VAL | A | 252 | 18.378 | 30.605 | 47.643 | 1.00 | 28.15 |
| ATOM | 1962 | CG2 | VAL | A | 252 | 16.614 | 32.234 | 48.405 | 1.00 | 30.93 |
| ATOM | 1963 | N   | TRP | A | 253 | 17.800 | 35.292 | 47.504 | 1.00 | 32.44 |
| ATOM | 1964 | CA  | TRP | A | 253 | 17.041 | 36.509 | 47.309 | 1.00 | 30.93 |
| ATOM | 1965 | C   | TRP | A | 253 | 17.468 | 37.341 | 46.119 | 1.00 | 43.56 |
| ATOM | 1966 | O   | TRP | A | 253 | 16.690 | 38.119 | 45.568 | 1.00 | 46.70 |
| ATOM | 1967 | CB  | TRP | A | 253 | 16.898 | 37.302 | 48.606 | 1.00 | 29.65 |
| ATOM | 1968 | CG  | TRP | A | 253 | 16.364 | 36.369 | 49.625 | 1.00 | 30.19 |
| ATOM | 1969 | CD1 | TRP | A | 253 | 17.086 | 35.546 | 50.413 | 1.00 | 32.81 |
| ATOM | 1970 | CD2 | TRP | A | 253 | 14.989 | 36.110 | 49.913 | 1.00 | 29.63 |
| ATOM | 1971 | NE1 | TRP | A | 253 | 16.251 | 34.794 | 51.194 | 1.00 | 30.69 |
| ATOM | 1972 | CE2 | TRP | A | 253 | 14.955 | 35.128 | 50.912 | 1.00 | 31.50 |
| ATOM | 1973 | CE3 | TRP | A | 253 | 13.789 | 36.637 | 49.450 | 1.00 | 30.18 |
| ATOM | 1974 | CZ2 | TRP | A | 253 | 13.746 | 34.657 | 51.433 | 1.00 | 30.31 |
| ATOM | 1975 | CZ3 | TRP | A | 253 | 12.600 | 36.164 | 49.958 | 1.00 | 31.14 |
| ATOM | 1976 | CH2 | TRP | A | 253 | 12.579 | 35.176 | 50.946 | 1.00 | 31.37 |
| ATOM | 1977 | N   | GLY | A | 254 | 18.697 | 37.182 | 45.675 | 1.00 | 42.35 |
| ATOM | 1978 | CA  | GLY | A | 254 | 19.101 | 37.944 | 44.509 | 1.00 | 41.34 |
| ATOM | 1979 | C   | GLY | A | 254 | 19.875 | 39.192 | 44.858 | 1.00 | 45.47 |
| ATOM | 1980 | O   | GLY | A | 254 | 21.079 | 39.236 | 44.671 | 1.00 | 45.89 |
| ATOM | 1981 | N   | GLN | A | 255 | 19.160 | 40.210 | 45.351 | 1.00 | 41.86 |
| ATOM | 1982 | CA  | GLN | A | 255 | 19.746 | 41.488 | 45.675 | 1.00 | 38.67 |
| ATOM | 1983 | C   | GLN | A | 255 | 19.576 | 41.776 | 47.153 | 1.00 | 40.18 |
| ATOM | 1984 | O   | GLN | A | 255 | 18.494 | 41.811 | 47.659 | 1.00 | 38.67 |
| ATOM | 1985 | CB  | GLN | A | 255 | 19.023 | 42.552 | 44.836 | 1.00 | 37.82 |
| ATOM | 1986 | CG  | GLN | A | 255 | 19.455 | 43.979 | 45.169 | 1.00 | 50.17 |
| ATOM | 1987 | CD  | GLN | A | 255 | 20.618 | 44.368 | 44.283 | 1.00 | 62.88 |
| ATOM | 1988 | OE1 | GLN | A | 255 | 21.104 | 43.612 | 43.463 | 1.00 | 55.76 |
| ATOM | 1989 | NE2 | GLN | A | 255 | 21.057 | 45.625 | 44.479 | 1.00 | 34.97 |
| ATOM | 1990 | N   | TYR | A | 256 | 20.716 | 41.900 | 47.866 | 1.00 | 33.01 |
| ATOM | 1991 | CA  | TYR | A | 256 | 20.651 | 42.361 | 49.258 | 1.00 | 28.69 |
| ATOM | 1992 | C   | TYR | A | 256 | 20.891 | 43.854 | 49.329 | 1.00 | 26.72 |
| ATOM | 1993 | O   | TYR | A | 256 | 21.963 | 44.321 | 49.225 | 1.00 | 24.22 |
| ATOM | 1994 | CB  | TYR | A | 256 | 21.743 | 41.629 | 50.075 | 1.00 | 29.99 |
| ATOM | 1995 | CG  | TYR | A | 256 | 21.567 | 41.867 | 51.556 | 1.00 | 35.47 |
| ATOM | 1996 | CD1 | TYR | A | 256 | 20.582 | 41.200 | 52.250 | 1.00 | 35.76 |
| ATOM | 1997 | CD2 | TYR | A | 256 | 22.405 | 42.746 | 52.239 | 1.00 | 37.52 |
| ATOM | 1998 | CE1 | TYR | A | 256 | 20.436 | 41.396 | 53.599 | 1.00 | 25.80 |
| ATOM | 1999 | CE2 | TYR | A | 256 | 22.255 | 42.946 | 53.588 | 1.00 | 39.10 |
| ATOM | 2000 | CZ  | TYR | A | 256 | 21.283 | 42.275 | 54.268 | 1.00 | 31.78 |
| ATOM | 2001 | OH  | TYR | A | 256 | 21.153 | 42.433 | 55.631 | 1.00 | 37.35 |
| ATOM | 2002 | N   | ASP | A | 257 | 19.834 | 44.613 | 49.463 | 1.00 | 23.26 |
| ATOM | 2003 | CA  |     |   |     |        |        |        |      |       |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 2022 | CB  | LEU | A | 259 | 16.500 | 50.809 | 53.693 | 1.00 | 27.63 |
| ATOM | 2023 | CG  | LEU | A | 259 | 15.706 | 51.980 | 54.298 | 1.00 | 31.51 |
| ATOM | 2024 | CD1 | LEU | A | 259 | 16.026 | 53.300 | 53.605 | 1.00 | 32.32 |
| ATOM | 2025 | CD2 | LEU | A | 259 | 14.212 | 51.731 | 54.253 | 1.00 | 26.87 |
| ATOM | 2026 | N   | VAL | A | 260 | 18.807 | 52.683 | 55.447 | 1.00 | 25.88 |
| ATOM | 2027 | CA  | VAL | A | 260 | 19.105 | 53.435 | 56.638 | 1.00 | 25.99 |
| ATOM | 2028 | C   | VAL | A | 260 | 17.896 | 54.336 | 56.796 | 1.00 | 34.83 |
| ATOM | 2029 | O   | VAL | A | 260 | 17.647 | 55.187 | 55.959 | 1.00 | 41.92 |
| ATOM | 2030 | CB  | VAL | A | 260 | 20.390 | 54.234 | 56.408 | 1.00 | 29.97 |
| ATOM | 2031 | CG1 | VAL | A | 260 | 20.701 | 55.179 | 57.592 | 1.00 | 32.08 |
| ATOM | 2032 | CG2 | VAL | A | 260 | 21.563 | 53.295 | 56.130 | 1.00 | 26.15 |
| ATOM | 2033 | N   | LEU | A | 261 | 17.098 | 54.120 | 57.815 | 1.00 | 28.41 |
| ATOM | 2034 | CA  | LEU | A | 261 | 15.865 | 54.878 | 58.024 | 1.00 | 25.52 |
| ATOM | 2035 | C   | LEU | A | 261 | 16.016 | 56.054 | 58.948 | 1.00 | 29.42 |
| ATOM | 2036 | O   | LEU | A | 261 | 17.090 | 56.300 | 59.489 | 1.00 | 29.96 |
| ATOM | 2037 | CB  | LEU | A | 261 | 14.874 | 53.921 | 58.706 | 1.00 | 25.70 |
| ATOM | 2038 | CG  | LEU | A | 261 | 14.387 | 52.877 | 57.740 | 1.00 | 33.14 |
| ATOM | 2039 | CD1 | LEU | A | 261 | 15.161 | 51.571 | 57.929 | 1.00 | 32.73 |
| ATOM | 2040 | CD2 | LEU | A | 261 | 12.900 | 52.686 | 57.935 | 1.00 | 43.74 |
| ATOM | 2041 | N   | PRO | A | 262 | 14.903 | 56.758 | 59.142 | 1.00 | 28.52 |
| ATOM | 2042 | CA  | PRO | A | 262 | 14.894 | 57.870 | 60.047 | 1.00 | 28.50 |
| ATOM | 2043 | C   | PRO | A | 262 | 15.152 | 57.294 | 61.432 | 1.00 | 35.36 |
| ATOM | 2044 | O   | PRO | A | 262 | 14.866 | 56.124 | 61.683 | 1.00 | 34.52 |
| ATOM | 2045 | CB  | PRO | A | 262 | 13.512 | 58.512 | 59.971 | 1.00 | 29.19 |
| ATOM | 2046 | CG  | PRO | A | 262 | 12.707 | 57.719 | 58.964 | 1.00 | 34.34 |
| ATOM | 2047 | CD  | PRO | A | 262 | 13.581 | 56.575 | 58.492 | 1.00 | 30.63 |
| ATOM | 2048 | N   | PRO | A | 263 | 15.706 | 58.105 | 62.327 | 1.00 | 31.50 |
| ATOM | 2049 | CA  | PRO | A | 263 | 16.060 | 57.657 | 63.673 | 1.00 | 28.77 |
| ATOM | 2050 | C   | PRO | A | 263 | 14.966 | 57.021 | 64.493 | 1.00 | 29.15 |
| ATOM | 2051 | O   | PRO | A | 263 | 15.256 | 56.335 | 65.434 | 1.00 | 26.36 |
| ATOM | 2052 | CB  | PRO | A | 263 | 16.652 | 58.867 | 64.392 | 1.00 | 29.16 |
| ATOM | 2053 | CG  | PRO | A | 263 | 16.851 | 59.954 | 63.335 | 1.00 | 31.55 |
| ATOM | 2054 | CD  | PRO | A | 263 | 15.994 | 59.558 | 62.138 | 1.00 | 29.17 |
| ATOM | 2055 | N   | SER | A | 264 | 13.712 | 57.258 | 64.143 | 1.00 | 33.87 |
| ATOM | 2056 | CA  | SER | A | 264 | 12.578 | 56.703 | 64.864 | 1.00 | 33.81 |
| ATOM | 2057 | C   | SER | A | 264 | 12.403 | 55.223 | 64.604 | 1.00 | 37.36 |
| ATOM | 2058 | O   | SER | A | 264 | 11.529 | 54.570 | 65.201 | 1.00 | 39.61 |
| ATOM | 2059 | CB  | SER | A | 264 | 11.280 | 57.423 | 64.576 | 1.00 | 35.61 |
| ATOM | 2060 | OG  | SER | A | 264 | 10.955 | 57.276 | 63.201 | 1.00 | 53.45 |
| ATOM | 2061 | N   | PHE | A | 265 | 13.213 | 54.684 | 63.710 | 1.00 | 29.00 |
| ATOM | 2062 | CA  | PHE | A | 265 | 13.136 | 53.256 | 63.453 | 1.00 | 28.56 |
| ATOM | 2063 | C   | PHE | A | 265 | 13.260 | 52.491 | 64.787 | 1.00 | 28.49 |
| ATOM | 2064 | O   | PHE | A | 265 | 14.208 | 52.675 | 65.533 | 1.00 | 27.36 |
| ATOM | 2065 | CB  | PHE | A | 265 | 14.200 | 52.833 | 62.454 | 1.00 | 31.40 |
| ATOM | 2066 | CG  | PHE | A | 265 | 13.875 | 51.458 | 62.028 | 1.00 | 34.51 |
| ATOM | 2067 | CD1 | PHE | A | 265 | 12.601 | 51.174 | 61.543 | 1.00 | 35.11 |
| ATOM | 2068 | CD2 | PHE | A | 265 | 14.814 | 50.435 | 62.156 | 1.00 | 38.94 |
| ATOM | 2069 | CE1 | PHE | A | 265 | 12.282 | 49.876 | 61.154 | 1.00 | 37.42 |
| ATOM | 2070 | CE2 | PHE | A | 265 | 14.511 | 49.131 | 61.772 | 1.00 | 42.65 |
| ATOM | 2071 | CZ  | PHE | A | 265 | 13.236 | 48.860 | 61.274 | 1.00 | 40.14 |
| ATOM | 2072 | N   | PRO | A | 266 | 12.272 | 51.650 | 65.128 | 1.00 | 24.06 |
| ATOM | 2073 | CA  | PRO | A | 266 | 12.249 | 50.945 | 66.419 | 1.00 | 20.62 |
| ATOM | 2074 | C   | PRO | A | 266 | 13.231 | 49.794 | 66.701 | 1.00 | 29.34 |
| ATOM | 2075 | O   | PRO | A | 266 | 13.343 | 49.364 | 67.847 | 1.00 | 28.17 |
| ATOM | 2076 | CB  | PRO | A | 266 | 10.808 | 50.463 | 66.593 | 1.00 | 19.16 |
| ATOM | 2077 | CG  | PRO | A | 266 | 10.076 | 50.686 | 65.281 | 1.00 | 21.07 |
| ATOM | 2078 | CD  | PRO | A | 266 | 11.046 | 51.355 | 64.325 | 1.00 | 19.44 |
| ATOM | 2079 | N   | TYR | A | 267 | 13.922 | 49.280 | 65.676 | 1.00 | 27.23 |
| ATOM | 2080 | CA  | TYR | A | 267 | 14.849 | 48.160 | 65.817 | 1.00 | 25.74 |
| ATOM | 2081 | C   | TYR | A | 267 | 16.181 | 48.454 | 65.189 | 1.00 | 32.57 |
| ATOM | 2082 | O   | TYR | A | 267 | 16.281 | 49.316 | 64.324 | 1.00 | 32.48 |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 2083 | CB  | TYR | A | 267 | 14.298 | 46.903 | 65.121 | 1.00 | 25.07 |
| ATOM | 2084 | CG  | TYR | A | 267 | 12.968 | 46.502 | 65.674 | 1.00 | 24.45 |
| ATOM | 2085 | CD1 | TYR | A | 267 | 12.915 | 45.765 | 66.856 | 1.00 | 27.05 |
| ATOM | 2086 | CD2 | TYR | A | 267 | 11.776 | 46.851 | 65.037 | 1.00 | 22.15 |
| ATOM | 2087 | CE1 | TYR | A | 267 | 11.697 | 45.387 | 67.419 | 1.00 | 25.01 |
| ATOM | 2088 | CE2 | TYR | A | 267 | 10.548 | 46.496 | 65.596 | 1.00 | 19.09 |
| ATOM | 2089 | CZ  | TYR | A | 267 | 10.510 | 45.767 | 66.786 | 1.00 | 17.98 |
| ATOM | 2090 | OH  | TYR | A | 267 | 9.302  | 45.416 | 67.353 | 1.00 | 19.51 |
| ATOM | 2091 | N   | GLY | A | 268 | 17.196 | 47.698 | 65.627 | 1.00 | 30.22 |
| ATOM | 2092 | CA  | GLY | A | 268 | 18.547 | 47.826 | 65.114 | 1.00 | 27.29 |
| ATOM | 2093 | C   | GLY | A | 268 | 18.485 | 47.620 | 63.614 | 1.00 | 29.82 |
| ATOM | 2094 | O   | GLY | A | 268 | 19.136 | 48.297 | 62.836 | 1.00 | 32.99 |
| ATOM | 2095 | N   | GLY | A | 269 | 17.637 | 46.676 | 63.228 | 1.00 | 23.19 |
| ATOM | 2096 | CA  | GLY | A | 269 | 17.393 | 46.320 | 61.853 | 1.00 | 21.62 |
| ATOM | 2097 | C   | GLY | A | 269 | 16.187 | 45.402 | 61.777 | 1.00 | 27.53 |
| ATOM | 2098 | O   | GLY | A | 269 | 15.681 | 44.948 | 62.820 | 1.00 | 20.14 |
| ATOM | 2099 | N   | MET | A | 270 | 15.735 | 45.154 | 60.528 | 1.00 | 27.81 |
| ATOM | 2100 | CA  | MET | A | 270 | 14.615 | 44.267 | 60.176 | 1.00 | 25.61 |
| ATOM | 2101 | C   | MET | A | 270 | 14.956 | 43.585 | 58.874 | 1.00 | 33.56 |
| ATOM | 2102 | O   | MET | A | 270 | 15.221 | 44.247 | 57.867 | 1.00 | 34.67 |
| ATOM | 2103 | CB  | MET | A | 270 | 13.247 | 44.936 | 60.028 | 1.00 | 26.07 |
| ATOM | 2104 | CG  | MET | A | 270 | 12.195 | 43.937 | 59.602 | 1.00 | 28.81 |
| ATOM | 2105 | SD  | MET | A | 270 | 11.875 | 42.742 | 60.929 | 1.00 | 37.39 |
| ATOM | 2106 | CE  | MET | A | 270 | 10.720 | 41.621 | 60.082 | 1.00 | 35.30 |
| ATOM | 2107 | N   | GLU | A | 271 | 14.995 | 42.263 | 58.904 | 1.00 | 32.20 |
| ATOM | 2108 | CA  | GLU | A | 271 | 15.393 | 41.459 | 57.753 | 1.00 | 33.32 |
| ATOM | 2109 | C   | GLU | A | 271 | 14.419 | 41.382 | 56.567 | 1.00 | 40.86 |
| ATOM | 2110 | O   | GLU | A | 271 | 14.087 | 40.285 | 56.107 | 1.00 | 42.02 |
| ATOM | 2111 | CB  | GLU | A | 271 | 15.802 | 40.054 | 58.230 | 1.00 | 35.05 |
| ATOM | 2112 | CG  | GLU | A | 271 | 14.607 | 39.218 | 58.760 | 1.00 | 33.55 |
| ATOM | 2113 | CD  | GLU | A | 271 | 14.291 | 39.428 | 60.219 | 1.00 | 25.52 |
| ATOM | 2114 | OE1 | GLU | A | 271 | 14.586 | 40.436 | 60.844 | 1.00 | 37.23 |
| ATOM | 2115 | OE2 | GLU | A | 271 | 13.699 | 38.393 | 60.757 | 1.00 | 25.86 |
| ATOM | 2116 | N   | ASN | A | 272 | 13.978 | 42.535 | 56.052 | 1.00 | 35.34 |
| ATOM | 2117 | CA  | ASN | A | 272 | 13.057 | 42.544 | 54.928 | 1.00 | 33.26 |
| ATOM | 2118 | C   | ASN | A | 272 | 13.787 | 42.048 | 53.702 | 1.00 | 34.47 |
| ATOM | 2119 | O   | ASN | A | 272 | 14.811 | 42.613 | 53.351 | 1.00 | 33.64 |
| ATOM | 2120 | CB  | ASN | A | 272 | 12.441 | 43.947 | 54.719 | 1.00 | 30.65 |
| ATOM | 2121 | CG  | ASN | A | 272 | 11.667 | 44.453 | 55.935 | 1.00 | 42.50 |
| ATOM | 2122 | OD1 | ASN | A | 272 | 11.908 | 45.554 | 56.475 | 1.00 | 47.09 |
| ATOM | 2123 | ND2 | ASN | A | 272 | 10.716 | 43.661 | 56.371 | 1.00 | 24.31 |
| ATOM | 2124 | N   | PRO | A | 273 | 13.281 | 40.983 | 53.078 | 1.00 | 29.63 |
| ATOM | 2125 | CA  | PRO | A | 273 | 13     |        |        |      |       |



005220 OF 22105

|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 2144 | CD2 | LEU | A | 275 | 13.712 | 48.478 | 50.554 | 1.00 | 31.48 |
| ATOM | 2145 | N   | THR | A | 276 | 17.062 | 45.244 | 53.570 | 1.00 | 29.67 |
| ATOM | 2146 | CA  | THR | A | 276 | 17.225 | 45.198 | 54.996 | 1.00 | 30.47 |
| ATOM | 2147 | C   | THR | A | 276 | 17.120 | 46.624 | 55.597 | 1.00 | 34.60 |
| ATOM | 2148 | O   | THR | A | 276 | 17.766 | 47.588 | 55.129 | 1.00 | 31.01 |
| ATOM | 2149 | CB  | THR | A | 276 | 18.508 | 44.397 | 55.387 | 1.00 | 30.98 |
| ATOM | 2150 | OG1 | THR | A | 276 | 18.224 | 43.030 | 55.512 | 1.00 | 42.01 |
| ATOM | 2151 | CG2 | THR | A | 276 | 19.124 | 44.835 | 56.694 | 1.00 | 29.43 |
| ATOM | 2152 | N   | PHE | A | 277 | 16.280 | 46.759 | 56.622 | 1.00 | 27.69 |
| ATOM | 2153 | CA  | PHE | A | 277 | 16.164 | 48.034 | 57.274 | 1.00 | 28.92 |
| ATOM | 2154 | C   | PHE | A | 277 | 17.184 | 48.065 | 58.403 | 1.00 | 36.07 |
| ATOM | 2155 | O   | PHE | A | 277 | 17.337 | 47.088 | 59.131 | 1.00 | 34.57 |
| ATOM | 2156 | CB  | PHE | A | 277 | 14.791 | 48.265 | 57.901 | 1.00 | 30.17 |
| ATOM | 2157 | CG  | PHE | A | 277 | 13.774 | 48.458 | 56.848 | 1.00 | 30.72 |
| ATOM | 2158 | CD1 | PHE | A | 277 | 14.011 | 47.966 | 55.568 | 1.00 | 30.73 |
| ATOM | 2159 | CD2 | PHE | A | 277 | 12.573 | 49.114 | 57.105 | 1.00 | 30.61 |
| ATOM | 2160 | CE1 | PHE | A | 277 | 13.072 | 48.135 | 54.552 | 1.00 | 29.30 |
| ATOM | 2161 | CE2 | PHE | A | 277 | 11.619 | 49.276 | 56.101 | 1.00 | 32.26 |
| ATOM | 2162 | CZ  | PHE | A | 277 | 11.862 | 48.772 | 54.824 | 1.00 | 27.48 |
| ATOM | 2163 | N   | VAL | A | 278 | 17.864 | 49.186 | 58.562 | 1.00 | 32.97 |
| ATOM | 2164 | CA  | VAL | A | 278 | 18.839 | 49.338 | 59.614 | 1.00 | 32.66 |
| ATOM | 2165 | C   | VAL | A | 278 | 18.696 | 50.698 | 60.248 | 1.00 | 37.01 |
| ATOM | 2166 | O   | VAL | A | 278 | 18.251 | 51.635 | 59.599 | 1.00 | 37.16 |
| ATOM | 2167 | CB  | VAL | A | 278 | 20.246 | 49.088 | 59.109 | 1.00 | 36.51 |
| ATOM | 2168 | CG1 | VAL | A | 278 | 20.173 | 47.967 | 58.086 | 1.00 | 37.40 |
| ATOM | 2169 | CG2 | VAL | A | 278 | 20.791 | 50.356 | 58.444 | 1.00 | 34.87 |
| ATOM | 2170 | N   | THR | A | 279 | 19.066 | 50.778 | 61.515 | 1.00 | 32.36 |
| ATOM | 2171 | CA  | THR | A | 279 | 18.948 | 51.994 | 62.264 | 1.00 | 31.03 |
| ATOM | 2172 | C   | THR | A | 279 | 20.121 | 52.883 | 62.035 | 1.00 | 37.42 |
| ATOM | 2173 | O   | THR | A | 279 | 21.243 | 52.397 | 61.920 | 1.00 | 39.87 |
| ATOM | 2174 | CB  | THR | A | 279 | 18.885 | 51.695 | 63.759 | 1.00 | 31.39 |
| ATOM | 2175 | OG1 | THR | A | 279 | 19.110 | 52.895 | 64.472 | 1.00 | 34.21 |
| ATOM | 2176 | CG2 | THR | A | 279 | 19.989 | 50.706 | 64.083 | 1.00 | 23.69 |
| ATOM | 2177 | N   | PRO | A | 280 | 19.845 | 54.187 | 62.000 | 1.00 | 30.07 |
| ATOM | 2178 | CA  | PRO | A | 280 | 20.903 | 55.132 | 61.802 | 1.00 | 27.00 |
| ATOM | 2179 | C   | PRO | A | 280 | 21.823 | 55.110 | 63.005 | 1.00 | 30.60 |
| ATOM | 2180 | O   | PRO | A | 280 | 22.951 | 55.588 | 62.934 | 1.00 | 30.20 |
| ATOM | 2181 | CB  | PRO | A | 280 | 20.249 | 56.497 | 61.601 | 1.00 | 26.23 |
| ATOM | 2182 | CG  | PRO | A | 280 | 18.769 | 56.337 | 61.889 | 1.00 | 28.07 |
| ATOM | 2183 | CD  | PRO | A | 280 | 18.499 | 54.848 | 61.984 | 1.00 | 26.11 |
| ATOM | 2184 | N   | THR | A | 281 | 21.348 | 54.509 | 64.112 | 1.00 | 27.82 |
| ATOM | 2185 | CA  | THR | A | 281 | 22.199 | 54.426 | 65.302 | 1.00 | 27.48 |
| ATOM | 2186 | C   | THR | A | 281 | 23.372 | 53.523 | 65.073 | 1.00 | 31.37 |
| ATOM | 2187 | O   | THR | A | 281 | 24.226 | 53.385 | 65.944 | 1.00 | 31.93 |
| ATOM | 2188 | CB  | THR | A | 281 | 21.499 | 54.016 | 66.601 | 1.00 | 21.45 |
| ATOM | 2189 | OG1 | THR | A | 281 | 21.021 | 52.681 | 66.524 | 1.00 | 33.18 |
| ATOM | 2190 | CG2 | THR | A | 281 | 20.388 | 54.994 | 66.874 | 1.00 | 9.89  |
| ATOM | 2191 | N   | LEU | A | 282 | 23.378 | 52.881 | 63.913 | 1.00 | 25.29 |
| ATOM | 2192 | CA  | LEU | A | 282 | 24.473 | 51.993 | 63.586 | 1.00 | 24.04 |
| ATOM | 2193 | C   | LEU | A | 282 | 25.682 | 52.790 | 63.049 | 1.00 | 34.74 |
| ATOM | 2194 | O   | LEU | A | 282 | 26.787 | 52.279 | 62.884 | 1.00 | 34.84 |
| ATOM | 2195 | CB  | LEU | A | 282 | 24.063 | 51.038 | 62.464 | 1.00 | 22.14 |
| ATOM | 2196 | CG  | LEU | A | 282 | 23.104 | 49.916 | 62.819 | 1.00 | 26.88 |
| ATOM | 2197 | CD1 | LEU | A | 282 | 23.312 | 48.809 | 61.791 | 1.00 | 27.77 |
| ATOM | 2198 | CD2 | LEU | A | 282 | 23.322 | 49.404 | 64.249 | 1.00 | 21.75 |
| ATOM | 2199 | N   | LEU | A | 283 | 25.465 | 54.063 | 62.744 | 1.00 | 32.05 |
| ATOM | 2200 | CA  | LEU | A | 283 | 26.501 | 54.903 | 62.159 | 1.00 | 31.43 |
| ATOM | 2201 | C   | LEU | A | 283 | 27.659 | 55.324 | 63.055 | 1.00 | 41.94 |
| ATOM | 2202 | O   | LEU | A | 283 | 27.907 | 56.525 | 63.196 | 1.00 | 49.19 |
| ATOM | 2203 | CB  | LEU | A | 283 | 25.861 | 56.117 | 61.418 | 1.00 | 29.55 |
| ATOM | 2204 | CG  | LEU | A | 283 | 24.720 | 55.661 | 60.488 | 1.00 | 32.94 |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 2205 | CD1 | LEU | A | 283 | 23.933 | 56.811 | 59.869 | 1.00 | 33.48 |
| ATOM | 2206 | CD2 | LEU | A | 283 | 25.232 | 54.716 | 59.409 | 1.00 | 28.39 |
| ATOM | 2207 | N   | ALA | A | 284 | 28.387 | 54.370 | 63.638 | 1.00 | 33.18 |
| ATOM | 2208 | CA  | ALA | A | 284 | 29.488 | 54.728 | 64.532 | 1.00 | 30.20 |
| ATOM | 2209 | C   | ALA | A | 284 | 30.655 | 55.492 | 63.922 | 1.00 | 31.97 |
| ATOM | 2210 | O   | ALA | A | 284 | 31.411 | 56.165 | 64.642 | 1.00 | 31.40 |
| ATOM | 2211 | CB  | ALA | A | 284 | 29.973 | 53.544 | 65.336 | 1.00 | 29.60 |
| ATOM | 2212 | N   | GLY | A | 285 | 30.801 | 55.371 | 62.605 | 1.00 | 27.10 |
| ATOM | 2213 | CA  | GLY | A | 285 | 31.882 | 56.018 | 61.867 | 1.00 | 29.77 |
| ATOM | 2214 | C   | GLY | A | 285 | 33.174 | 55.194 | 61.910 | 1.00 | 39.25 |
| ATOM | 2215 | O   | GLY | A | 285 | 34.264 | 55.649 | 61.544 | 1.00 | 41.2  |
| ATOM | 2216 | N   | ASP | A | 286 | 33.022 | 53.951 | 62.363 | 1.00 | 34.57 |
| ATOM | 2217 | CA  | ASP | A | 286 | 34.144 | 53.057 | 62.473 | 1.00 | 32.57 |
| ATOM | 2218 | C   | ASP | A | 286 | 33.805 | 51.625 | 62.130 | 1.00 | 31.59 |
| ATOM | 2219 | O   | ASP | A | 286 | 34.609 | 50.743 | 62.325 | 1.00 | 29.27 |
| ATOM | 2220 | CB  | ASP | A | 286 | 34.812 | 53.163 | 63.860 | 1.00 | 34.65 |
| ATOM | 2221 | CG  | ASP | A | 286 | 34.081 | 52.447 | 64.945 | 1.00 | 41.93 |
| ATOM | 2222 | OD1 | ASP | A | 286 | 33.008 | 51.893 | 64.765 | 1.00 | 45.21 |
| ATOM | 2223 | OD2 | ASP | A | 286 | 34.714 | 52.492 | 66.087 | 1.00 | 35.67 |
| ATOM | 2224 | N   | LYS | A | 287 | 32.590 | 51.395 | 61.641 | 1.00 | 29.46 |
| ATOM | 2225 | CA  | LYS | A | 287 | 32.199 | 50.038 | 61.272 | 1.00 | 31.62 |
| ATOM | 2226 | C   | LYS | A | 287 | 31.976 | 49.060 | 62.437 | 1.00 | 37.91 |
| ATOM | 2227 | O   | LYS | A | 287 | 31.761 | 47.879 | 62.240 | 1.00 | 37.91 |
| ATOM | 2228 | CB  | LYS | A | 287 | 33.215 | 49.447 | 60.304 | 1.00 | 32.17 |
| ATOM | 2229 | CG  | LYS | A | 287 | 33.510 | 50.358 | 59.119 | 1.00 | 51.60 |
| ATOM | 2230 | CD  | LYS | A | 287 | 33.960 | 49.601 | 57.877 | 1.00 | 50.74 |
| ATOM | 2231 | CE  | LYS | A | 287 | 35.290 | 50.105 | 57.328 | 1.00 | 63.80 |
| ATOM | 2232 | NZ  | LYS | A | 287 | 35.167 | 50.866 | 56.069 | 1.00 | 71.91 |
| ATOM | 2233 | N   | SER | A | 288 | 32.168 | 49.575 | 63.647 | 1.00 | 31.58 |
| ATOM | 2234 | CA  | SER | A | 288 | 32.079 | 48.737 | 64.810 | 1.00 | 27.15 |
| ATOM | 2235 | C   | SER | A | 288 | 30.742 | 48.137 | 65.142 | 1.00 | 36.08 |
| ATOM | 2236 | O   | SER | A | 288 | 30.676 | 47.318 | 66.057 | 1.00 | 37.87 |
| ATOM | 2237 | CB  | SER | A | 288 | 32.618 | 49.463 | 66.005 | 1.00 | 16.31 |
| ATOM | 2238 | OG  | SER | A | 288 | 31.659 | 50.443 | 66.312 | 1.00 | 29.71 |
| ATOM | 2239 | N   | LEU | A | 289 | 29.669 | 48.529 | 64.460 | 1.00 | 29.34 |
| ATOM | 2240 | CA  | LEU | A | 289 | 28.351 | 47.979 | 64.794 | 1.00 | 24.70 |
| ATOM | 2241 | C   | LEU | A | 289 | 27.792 | 47.105 | 63.686 | 1.00 | 32.97 |
| ATOM | 2242 | O   | LEU | A | 289 | 26.591 | 46.766 | 63.648 | 1.00 | 30.35 |
| ATOM | 2243 | CB  | LEU | A | 289 | 27.385 | 49.090 | 65.191 | 1.00 | 21.45 |
| ATOM | 2244 | CG  | LEU | A | 289 | 27.954 | 49.887 | 66.347 | 1.00 | 22.99 |
| ATOM | 2245 | CD1 | LEU | A | 289 | 26.881 | 50.769 | 66.950 | 1.00 | 20.66 |
| ATOM | 2246 | CD2 | LEU | A | 289 | 28.381 | 48.881 | 67.394 | 1.00 | 29.65 |
| ATOM | 2247 | N   | SER | A | 290 | 28.723 |        |        |      |       |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 2266 | CG1 | VAL | A | 292 | 21.877 | 45.486 | 62.946 | 1.00 | 33.48 |
| ATOM | 2267 | CG2 | VAL | A | 292 | 23.328 | 45.478 | 65.014 | 1.00 | 35.02 |
| ATOM | 2268 | N   | ILE | A | 293 | 24.653 | 43.975 | 60.861 | 1.00 | 27.92 |
| ATOM | 2269 | CA  | ILE | A | 293 | 24.527 | 43.685 | 59.461 | 1.00 | 28.71 |
| ATOM | 2270 | C   | ILE | A | 293 | 24.658 | 42.159 | 59.296 | 1.00 | 35.03 |
| ATOM | 2271 | O   | ILE | A | 293 | 23.860 | 41.475 | 58.624 | 1.00 | 38.34 |
| ATOM | 2272 | CB  | ILE | A | 293 | 25.554 | 44.438 | 58.606 | 1.00 | 33.84 |
| ATOM | 2273 | CG1 | ILE | A | 293 | 25.608 | 45.952 | 58.898 | 1.00 | 34.55 |
| ATOM | 2274 | CG2 | ILE | A | 293 | 25.305 | 44.186 | 57.121 | 1.00 | 36.50 |
| ATOM | 2275 | CD1 | ILE | A | 293 | 24.265 | 46.680 | 58.808 | 1.00 | 30.49 |
| ATOM | 2276 | N   | ALA | A | 294 | 25.668 | 41.584 | 59.934 | 1.00 | 23.76 |
| ATOM | 2277 | CA  | ALA | A | 294 | 25.836 | 40.138 | 59.809 | 1.00 | 19.95 |
| ATOM | 2278 | C   | ALA | A | 294 | 24.559 | 39.409 | 60.165 | 1.00 | 27.33 |
| ATOM | 2279 | O   | ALA | A | 294 | 24.183 | 38.422 | 59.505 | 1.00 | 25.48 |
| ATOM | 2280 | CB  | ALA | A | 294 | 26.984 | 39.644 | 60.688 | 1.00 | 19.24 |
| ATOM | 2281 | N   | HIS | A | 295 | 23.917 | 39.934 | 61.244 | 1.00 | 27.63 |
| ATOM | 2282 | CA  | HIS | A | 295 | 22.666 | 39.414 | 61.797 | 1.00 | 26.83 |
| ATOM | 2283 | C   | HIS | A | 295 | 21.611 | 39.383 | 60.734 | 1.00 | 28.61 |
| ATOM | 2284 | O   | HIS | A | 295 | 21.169 | 38.301 | 60.348 | 1.00 | 25.72 |
| ATOM | 2285 | CB  | HIS | A | 295 | 22.148 | 40.175 | 63.028 | 1.00 | 27.98 |
| ATOM | 2286 | CG  | HIS | A | 295 | 20.937 | 39.534 | 63.657 | 1.00 | 31.62 |
| ATOM | 2287 | ND1 | HIS | A | 295 | 21.047 | 38.675 | 64.763 | 1.00 | 32.66 |
| ATOM | 2288 | CD2 | HIS | A | 295 | 19.602 | 39.643 | 63.338 | 1.00 | 30.92 |
| ATOM | 2289 | CE1 | HIS | A | 295 | 19.802 | 38.298 | 65.088 | 1.00 | 30.14 |
| ATOM | 2290 | NE2 | HIS | A | 295 | 18.916 | 38.860 | 64.254 | 1.00 | 30.24 |
| ATOM | 2291 | N   | GLU | A | 296 | 21.257 | 40.590 | 60.251 | 1.00 | 27.23 |
| ATOM | 2292 | CA  | GLU | A | 296 | 20.266 | 40.749 | 59.195 | 1.00 | 25.98 |
| ATOM | 2293 | C   | GLU | A | 296 | 20.533 | 39.790 | 58.056 | 1.00 | 32.73 |
| ATOM | 2294 | O   | GLU | A | 296 | 19.628 | 39.081 | 57.561 | 1.00 | 31.88 |
| ATOM | 2295 | CB  | GLU | A | 296 | 20.046 | 42.203 | 58.728 | 1.00 | 24.55 |
| ATOM | 2296 | CG  | GLU | A | 296 | 19.892 | 43.148 | 59.936 | 1.00 | 23.16 |
| ATOM | 2297 | CD  | GLU | A | 296 | 18.939 | 42.632 | 60.991 | 1.00 | 53.50 |
| ATOM | 2298 | OE1 | GLU | A | 296 | 17.964 | 41.956 | 60.700 | 1.00 | 23.99 |
| ATOM | 2299 | OE2 | GLU | A | 296 | 19.237 | 43.006 | 62.233 | 1.00 | 32.77 |
| ATOM | 2300 | N   | ILE | A | 297 | 21.803 | 39.745 | 57.675 | 1.00 | 25.37 |
| ATOM | 2301 | CA  | ILE | A | 297 | 22.195 | 38.870 | 56.599 | 1.00 | 22.64 |
| ATOM | 2302 | C   | ILE | A | 297 | 21.812 | 37.445 | 56.859 | 1.00 | 27.47 |
| ATOM | 2303 | O   | ILE | A | 297 | 21.175 | 36.799 | 56.048 | 1.00 | 26.25 |
| ATOM | 2304 | CB  | ILE | A | 297 | 23.672 | 38.963 | 56.302 | 1.00 | 24.19 |
| ATOM | 2305 | CG1 | ILE | A | 297 | 23.920 | 40.140 | 55.355 | 1.00 | 25.28 |
| ATOM | 2306 | CG2 | ILE | A | 297 | 24.079 | 37.686 | 55.626 | 1.00 | 20.77 |
| ATOM | 2307 | CD1 | ILE | A | 297 | 25.325 | 40.705 | 55.435 | 1.00 | 16.26 |
| ATOM | 2308 | N   | SER | A | 298 | 22.226 |        |        |      |       |



|      |      |     |     |   |       |        |        |        |      |       |
|------|------|-----|-----|---|-------|--------|--------|--------|------|-------|
| ATOM | 2327 | O   | SER | A | 300   | 17.075 | 33.463 | 54.305 | 1.00 | 33.28 |
| ATOM | 2328 | CB  | SER | A | 300   | 18.941 | 36.092 | 53.965 | 1.00 | 27.31 |
| ATOM | 2329 | OG  | SER | A | 300   | 18.947 | 37.519 | 53.962 | 1.00 | 49.96 |
| ATOM | 2330 | N   | TRP | A | 301   | 18.773 | 33.411 | 55.752 | 1.00 | 33.09 |
| ATOM | 2331 | CA  | TRP | A | 301   | 18.702 | 31.969 | 55.829 | 1.00 | 31.84 |
| ATOM | 2332 | C   | TRP | A | 301   | 17.740 | 31.511 | 56.895 | 1.00 | 32.15 |
| ATOM | 2333 | O   | TRP | A | 301   | 16.764 | 30.876 | 56.620 | 1.00 | 27.05 |
| ATOM | 2334 | CB  | TRP | A | 301   | 20.095 | 31.429 | 56.082 | 1.00 | 30.16 |
| ATOM | 2335 | CG  | TRP | A | 301   | 20.791 | 31.421 | 54.801 | 1.00 | 32.02 |
| ATOM | 2336 | CD1 | TRP | A | 301   | 20.787 | 30.393 | 53.859 | 1.00 | 35.05 |
| ATOM | 2337 | CD2 | TRP | A | 301   | 21.496 | 32.520 | 54.202 | 1.00 | 30.84 |
| ATOM | 2338 | NE1 | TRP | A | 301   | 21.415 | 30.732 | 52.722 | 1.00 | 33.29 |
| ATOM | 2339 | CE2 | TRP | A | 301   | 21.886 | 32.112 | 52.921 | 1.00 | 33.44 |
| ATOM | 2340 | CE3 | TRP | A | 301   | 21.811 | 33.790 | 54.631 | 1.00 | 32.65 |
| ATOM | 2341 | CZ2 | TRP | A | 301   | 22.577 | 32.970 | 52.108 | 1.00 | 32.21 |
| ATOM | 2342 | CZ3 | TRP | A | 301   | 22.503 | 34.652 | 53.812 | 1.00 | 36.10 |
| ATOM | 2343 | CH2 | TRP | A | 301   | 22.888 | 34.239 | 52.544 | 1.00 | 36.83 |
| ATOM | 2344 | N   | THR | A | 302   | 18.042 | 31.864 | 58.146 | 1.00 | 31.77 |
| ATOM | 2345 | CA  | THR | A | 302   | 17.125 | 31.488 | 59.215 | 1.00 | 33.55 |
| ATOM | 2346 | C   | THR | A | 302   | 16.276 | 32.690 | 59.695 | 1.00 | 36.35 |
| ATOM | 2347 | O   | THR | A | 302   | 16.759 | 33.590 | 60.330 | 1.00 | 36.56 |
| ATOM | 2348 | CB  | THR | A | 302   | 17.963 | 30.920 | 60.366 | 1.00 | 31.04 |
| ATOM | 2349 | OG1 | THR | A | 302   | 19.047 | 31.807 | 60.639 | 1.00 | 38.50 |
| ATOM | 2350 | CG2 | THR | A | 302   | 18.544 | 29.555 | 59.967 | 1.00 | 17.10 |
| ATOM | 2351 | N   | GLY | A | 303   | 15.053 | 32.418 | 59.250 | 1.00 | 25.28 |
| ATOM | 2352 | CA  | GLY | A | 303   | 13.908 | 33.236 | 59.483 | 1.00 | 21.59 |
| ATOM | 2353 | C   | GLY | A | 303   | 13.202 | 33.382 | 58.163 | 1.00 | 26.99 |
| ATOM | 2354 | O   | GLY | A | 303   | 12.040 | 33.040 | 57.994 | 1.00 | 26.18 |
| ATOM | 2355 | N   | ASN | A | 304   | 13.936 | 33.891 | 57.195 | 1.00 | 28.05 |
| ATOM | 2356 | CA  | ASN | A | 304   | 13.363 | 34.101 | 55.875 | 1.00 | 28.17 |
| ATOM | 2357 | C   | ASN | A | 304   | 13.141 | 32.839 | 55.056 | 1.00 | 28.99 |
| ATOM | 2358 | O   | ASN | A | 304   | 12.118 | 32.715 | 54.415 | 1.00 | 24.87 |
| ATOM | 2359 | CB  | ASN | A | 304   | 14.091 | 35.176 | 55.047 | 1.00 | 23.55 |
| ATOM | 2360 | CG  | ASN | A | 304   | 14.133 | 36.499 | 55.757 | 1.00 | 37.80 |
| ATOM | 2361 | OD1 | ASN | A | 304   | 13.630 | 36.613 | 56.892 | 1.00 | 20.66 |
| ATOM | 2362 | ND2 | ASN | A | 304   | 14.752 | 37.488 | 55.093 | 1.00 | 24.17 |
| ATOM | 2363 | N   | LEU | A | 305   | 14.110 | 31.919 | 55.055 | 1.00 | 27.24 |
| ATOM | 2364 | CA  | LEU | A | 305   | 13.987 | 30.677 | 54.306 | 1.00 | 27.34 |
| ATOM | 2365 | C   | LEU | A | 305   | 13.218 | 29.665 | 55.121 | 1.00 | 31.29 |
| ATOM | 2366 | O   | LEU | A | 305   | 12.235 | 29.051 | 54.678 | 1.00 | 29.23 |
| ATOM | 2367 | CB  | LEU | A | 305   | 15.371 | 30.119 | 53.967 | 1.00 | 27.62 |
| ATOM | 2368 | CG  | LEU | A | 305   | 15.805 | 30.593 | 52.603 | 1.00 | 32.23 |
| ATOM | 2369 | CD1 | LEU | A | 305</ |        |        |        |      |       |



|      |      |     |           |        |        |        |      |       |
|------|------|-----|-----------|--------|--------|--------|------|-------|
| ATOM | 2388 | O   | ASN A 308 | 7.072  | 30.535 | 61.450 | 1.00 | 32.96 |
| ATOM | 2389 | CB  | ASN A 308 | 9.194  | 30.790 | 63.972 | 1.00 | 23.57 |
| ATOM | 2390 | CG  | ASN A 308 | 8.935  | 32.298 | 63.745 | 1.00 | 30.38 |
| ATOM | 2391 | OD1 | ASN A 308 | 9.505  | 33.190 | 64.400 | 1.00 | 23.70 |
| ATOM | 2392 | ND2 | ASN A 308 | 8.056  | 32.608 | 62.818 | 1.00 | 41.34 |
| ATOM | 2393 | N   | LYS A 309 | 6.890  | 28.658 | 62.640 | 1.00 | 24.10 |
| ATOM | 2394 | CA  | LYS A 309 | 5.502  | 28.433 | 62.230 | 1.00 | 23.40 |
| ATOM | 2395 | C   | LYS A 309 | 4.514  | 29.380 | 62.964 | 1.00 | 28.17 |
| ATOM | 2396 | O   | LYS A 309 | 3.430  | 29.756 | 62.474 | 1.00 | 22.88 |
| ATOM | 2397 | CB  | LYS A 309 | 5.151  | 26.975 | 62.459 | 1.00 | 24.26 |
| ATOM | 2398 | CG  | LYS A 309 | 4.036  | 26.478 | 61.555 | 1.00 | 28.57 |
| ATOM | 2399 | CD  | LYS A 309 | 3.543  | 25.075 | 61.924 | 1.00 | 38.25 |
| ATOM | 2400 | CE  | LYS A 309 | 3.475  | 24.112 | 60.739 | 1.00 | 78.39 |
| ATOM | 2401 | NZ  | LYS A 309 | 4.389  | 22.953 | 60.849 | 1.00 | 98.22 |
| ATOM | 2402 | N   | THR A 310 | 4.917  | 29.744 | 64.179 | 1.00 | 23.46 |
| ATOM | 2403 | CA  | THR A 310 | 4.179  | 30.616 | 65.037 | 1.00 | 22.98 |
| ATOM | 2404 | C   | THR A 310 | 5.142  | 31.336 | 65.922 | 1.00 | 31.43 |
| ATOM | 2405 | O   | THR A 310 | 6.223  | 30.836 | 66.230 | 1.00 | 31.51 |
| ATOM | 2406 | CB  | THR A 310 | 3.104  | 29.917 | 65.871 | 1.00 | 34.01 |
| ATOM | 2407 | OG1 | THR A 310 | 3.684  | 29.148 | 66.945 | 1.00 | 27.97 |
| ATOM | 2408 | CG2 | THR A 310 | 2.174  | 29.114 | 64.956 | 1.00 | 24.58 |
| ATOM | 2409 | N   | TRP A 311 | 4.733  | 32.527 | 66.299 | 1.00 | 29.82 |
| ATOM | 2410 | CA  | TRP A 311 | 5.559  | 33.371 | 67.120 | 1.00 | 30.49 |
| ATOM | 2411 | C   | TRP A 311 | 6.044  | 32.692 | 68.381 | 1.00 | 26.99 |
| ATOM | 2412 | O   | TRP A 311 | 7.015  | 33.101 | 68.971 | 1.00 | 25.15 |
| ATOM | 2413 | CB  | TRP A 311 | 4.933  | 34.768 | 67.320 | 1.00 | 30.34 |
| ATOM | 2414 | CG  | TRP A 311 | 4.706  | 35.412 | 66.001 | 1.00 | 30.63 |
| ATOM | 2415 | CD1 | TRP A 311 | 3.514  | 35.785 | 65.490 | 1.00 | 32.07 |
| ATOM | 2416 | CD2 | TRP A 311 | 5.705  | 35.723 | 65.008 | 1.00 | 31.31 |
| ATOM | 2417 | NE1 | TRP A 311 | 3.703  | 36.335 | 64.250 | 1.00 | 29.97 |
| ATOM | 2418 | CE2 | TRP A 311 | 5.033  | 36.317 | 63.931 | 1.00 | 32.88 |
| ATOM | 2419 | CE3 | TRP A 311 | 7.099  | 35.586 | 64.943 | 1.00 | 31.44 |
| ATOM | 2420 | CZ2 | TRP A 311 | 5.721  | 36.771 | 62.804 | 1.00 | 31.56 |
| ATOM | 2421 | CZ3 | TRP A 311 | 7.779  | 36.059 | 63.848 | 1.00 | 30.39 |
| ATOM | 2422 | CH2 | TRP A 311 | 7.089  | 36.639 | 62.789 | 1.00 | 30.58 |
| ATOM | 2423 | N   | ASP A 312 | 5.366  | 31.632 | 68.770 | 1.00 | 27.36 |
| ATOM | 2424 | CA  | ASP A 312 | 5.757  | 30.868 | 69.950 | 1.00 | 27.38 |
| ATOM | 2425 | C   | ASP A 312 | 7.149  | 30.213 | 69.757 | 1.00 | 31.25 |
| ATOM | 2426 | O   | ASP A 312 | 7.826  | 29.802 | 70.718 | 1.00 | 27.07 |
| ATOM | 2427 | CB  | ASP A 312 | 4.697  | 29.750 | 70.217 | 1.00 | 25.96 |
| ATOM | 2428 | CG  | ASP A 312 | 3.432  | 30.230 | 70.872 | 1.00 | 27.42 |
| ATOM | 2429 | OD1 | ASP A 312 | 3.197  | 31.396 | 71.102 | 1.00 | 28.97 |
| ATOM | 2430 | OD2 | ASP A 312 | 2.623  | 29.265 | 71.208 | 1.00 | 29.33 |
| ATOM | 2431 | N   | HIS A 313 | 7.562  | 30.089 | 68.487 | 1.00 | 25.04 |
| ATOM | 2432 | CA  | HIS A 313 | 8.820  | 29.454 | 68.164 | 1.00 | 23.48 |
| ATOM | 2433 | C   | HIS A 313 | 9.864  | 30.452 | 67.737 | 1.00 | 25.38 |
| ATOM | 2434 | O   | HIS A 313 | 10.929 | 30.139 | 67.214 | 1.00 | 29.97 |
| ATOM | 2435 | CB  | HIS A 313 | 8.588  | 28.245 | 67.209 | 1.00 | 25.00 |
| ATOM | 2436 | CG  | HIS A 313 | 7.641  | 27.230 | 67.837 | 1.00 | 29.77 |
| ATOM | 2437 | ND1 | HIS A 313 | 8.087  | 26.183 | 68.635 | 1.00 | 31.37 |
| ATOM | 2438 | CD2 | HIS A 313 | 6.279  | 27.152 | 67.808 | 1.00 | 31.31 |
| ATOM | 2439 | CE1 | HIS A 313 | 7.015  | 25.509 | 69.039 | 1.00 | 28.91 |
| ATOM | 2440 | NE2 | HIS A 313 | 5.913  | 26.066 | 68.559 | 1.00 | 29.40 |
| ATOM | 2441 | N   | PHE A 314 | 9.521  | 31.682 | 68.005 | 1.00 | 17.43 |
| ATOM | 2442 | CA  | PHE A 314 | 10.345 | 32.810 | 67.701 | 1.00 | 17.16 |
| ATOM | 2443 | C   | PHE A 314 | 11.852 | 32.523 | 67.812 | 1.00 | 26.01 |
| ATOM | 2444 | O   | PHE A 314 | 12.669 | 32.922 | 66.963 | 1.00 | 30.40 |
| ATOM | 2445 | CB  | PHE A 314 | 9.908  | 34.056 | 68.517 | 1.00 | 18.63 |
| ATOM | 2446 | CG  | PHE A 314 | 10.592 | 35.351 | 68.113 | 1.00 | 20.10 |
| ATOM | 2447 | CD1 | PHE A 314 | 10.712 | 35.697 | 66.768 | 1.00 | 21.80 |
| ATOM | 2448 | CD2 | PHE A 314 | 11.129 | 36.214 | 69.070 | 1.00 | 22.60 |



|      |      |     |       |   |     |        |        |        |      |       |
|------|------|-----|-------|---|-----|--------|--------|--------|------|-------|
| ATOM | 2449 | CE1 | PHE   | A | 314 | 11.337 | 36.890 | 66.400 | 1.00 | 24.74 |
| ATOM | 2450 | CE2 | PHE   | A | 314 | 11.750 | 37.416 | 68.716 | 1.00 | 27.24 |
| ATOM | 2451 | CZ  | PHE   | A | 314 | 11.857 | 37.756 | 67.368 | 1.00 | 24.97 |
| ATOM | 2452 | N   | TRP   | A | 315 | 12.235 | 31.828 | 68.861 | 1.00 | 19.66 |
| ATOM | 2453 | CA  | TRP   | A | 315 | 13.639 | 31.541 | 69.068 | 1.00 | 17.87 |
| ATOM | 2454 | C   | TRP   | A | 315 | 14.292 | 30.775 | 67.953 | 1.00 | 28.55 |
| ATOM | 2455 | O   | TRP   | A | 315 | 15.518 | 30.769 | 67.830 | 1.00 | 29.23 |
| ATOM | 2456 | CB  | TRP   | A | 315 | 13.860 | 30.842 | 70.362 | 1.00 | 16.03 |
| ATOM | 2457 | CG  | TRP   | A | 315 | 13.613 | 29.408 | 70.161 | 1.00 | 19.64 |
| ATOM | 2458 | CD1 | TRP   | A | 315 | 12.428 | 28.787 | 70.247 | 1.00 | 22.39 |
| ATOM | 2459 | CD2 | TRP   | A | 315 | 14.599 | 28.430 | 69.876 | 1.00 | 21.70 |
| ATOM | 2460 | NE1 | TRP   | A | 315 | 12.597 | 27.457 | 70.033 | 1.00 | 24.22 |
| ATOM | 2461 | CE2 | TRP   | A | 315 | 13.934 | 27.205 | 69.801 | 1.00 | 27.96 |
| ATOM | 2462 | CE3 | TRP   | A | 315 | 15.976 | 28.481 | 69.681 | 1.00 | 22.89 |
| ATOM | 2463 | CZ2 | TRP   | A | 315 | 14.631 | 26.018 | 69.547 | 1.00 | 27.76 |
| ATOM | 2464 | CZ3 | TRP   | A | 315 | 16.651 | 27.321 | 69.421 | 1.00 | 23.16 |
| ATOM | 2465 | CH2 | TRP   | A | 315 | 15.991 | 26.108 | 69.341 | 1.00 | 23.94 |
| ATOM | 2466 | N   | LEU   | A | 316 | 13.488 | 30.114 | 67.144 | 1.00 | 26.33 |
| ATOM | 2467 | CA  | LEU   | A | 316 | 14.092 | 29.400 | 66.067 | 1.00 | 25.44 |
| ATOM | 2468 | C   | LEU   | A | 316 | 14.666 | 30.443 | 65.129 | 1.00 | 33.21 |
| ATOM | 2469 | O   | LEU   | A | 316 | 15.737 | 30.252 | 64.530 | 1.00 | 37.80 |
| ATOM | 2470 | CB  | LEU   | A | 316 | 13.050 | 28.567 | 65.311 | 1.00 | 24.82 |
| ATOM | 2471 | CG  | LEU   | A | 316 | 12.663 | 27.242 | 65.956 | 1.00 | 27.62 |
| ATOM | 2472 | CD1 | LEU   | A | 316 | 11.574 | 26.552 | 65.106 | 1.00 | 22.30 |
| ATOM | 2473 | CD2 | LEU   | A | 316 | 13.897 | 26.344 | 66.097 | 1.00 | 27.03 |
| ATOM | 2474 | N   | ASN   | A | 317 | 13.931 | 31.555 | 64.997 | 1.00 | 20.55 |
| ATOM | 2475 | CA  | ASN   | A | 317 | 14.354 | 32.624 | 64.115 | 1.00 | 19.34 |
| ATOM | 2476 | C   | ASN   | A | 317 | 15.603 | 33.333 | 64.531 | 1.00 | 30.38 |
| ATOM | 2477 | O   | ASN   | A | 317 | 16.553 | 33.425 | 63.766 | 1.00 | 32.04 |
| ATOM | 2478 | CB  | ASN   | A | 317 | 13.273 | 33.682 | 63.838 | 1.00 | 14.82 |
| ATOM | 2479 | CG  | ASN   | A | 317 | 12.330 | 33.177 | 62.793 | 1.00 | 31.14 |
| ATOM | 2480 | OD1 | ASN   | A | 317 | 12.151 | 31.966 | 62.657 | 1.00 | 38.42 |
| ATOM | 2481 | ND2 | ASN   | A | 317 | 11.724 | 34.074 | 62.049 | 1.00 | 17.34 |
| ATOM | 2482 | N   | GLU   | A | 318 | 15.562 | 33.870 | 65.750 | 1.00 | 26.15 |
| ATOM | 2483 | CA  | GLU   | A | 318 | 16.624 | 34.648 | 66.358 | 1.00 | 20.23 |
| ATOM | 2484 | C   | GLU   | A | 318 | 17.860 | 33.884 | 66.816 | 1.00 | 23.53 |
| ATOM | 2485 | O   | GLU   | A | 318 | 19.006 | 34.273 | 66.554 | 1.00 | 26.34 |
| ATOM | 2486 | CB  | GLU   | A | 318 | 15.998 | 35.484 | 67.456 | 1.00 | 19.11 |
| ATOM | 2487 | CG  | GLU   | A | 318 | 14.999 | 36.480 | 66.800 | 1.00 | 24.06 |
| ATOM | 2488 | CD  | GLU   | A | 318 | 15.615 | 37.391 | 65.758 | 1.00 | 40.32 |
| ATOM | 2489 | OE1 | GLU   | A | 318 | 16.833 | 37.559 | 65.612 | 1.00 | 21.24 |
| ATOM | 2490 | OE2 | GLU   | A | 318 | 14.703 | 38.025 | 65.062 | 1.00 | 24.23 |
| ATOM | 2491 | N   | GLY</ |   |     |        |        |        |      |       |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 2510 | OG1 | THR | A | 321 | 18.403 | 34.392 | 62.523 | 1.00 | 27.92 |
| ATOM | 2511 | CG2 | THR | A | 321 | 19.999 | 36.088 | 62.087 | 1.00 | 18.05 |
| ATOM | 2512 | N   | VAL | A | 322 | 21.496 | 34.634 | 65.659 | 1.00 | 21.90 |
| ATOM | 2513 | CA  | VAL | A | 322 | 22.610 | 35.054 | 66.470 | 1.00 | 19.44 |
| ATOM | 2514 | C   | VAL | A | 322 | 23.762 | 34.071 | 66.285 | 1.00 | 24.43 |
| ATOM | 2515 | O   | VAL | A | 322 | 24.926 | 34.414 | 66.188 | 1.00 | 21.48 |
| ATOM | 2516 | CB  | VAL | A | 322 | 22.218 | 35.185 | 67.928 | 1.00 | 20.92 |
| ATOM | 2517 | CG1 | VAL | A | 322 | 23.406 | 35.644 | 68.772 | 1.00 | 18.37 |
| ATOM | 2518 | CG2 | VAL | A | 322 | 21.093 | 36.200 | 68.048 | 1.00 | 20.01 |
| ATOM | 2519 | N   | TYR | A | 323 | 23.427 | 32.811 | 66.197 | 1.00 | 27.08 |
| ATOM | 2520 | CA  | TYR | A | 323 | 24.446 | 31.803 | 66.013 | 1.00 | 26.26 |
| ATOM | 2521 | C   | TYR | A | 323 | 25.222 | 32.036 | 64.728 | 1.00 | 28.26 |
| ATOM | 2522 | O   | TYR | A | 323 | 26.431 | 31.894 | 64.643 | 1.00 | 27.51 |
| ATOM | 2523 | CB  | TYR | A | 323 | 23.804 | 30.407 | 66.020 | 1.00 | 25.74 |
| ATOM | 2524 | CG  | TYR | A | 323 | 24.867 | 29.341 | 65.987 | 1.00 | 26.66 |
| ATOM | 2525 | CD1 | TYR | A | 323 | 25.539 | 28.957 | 67.150 | 1.00 | 29.09 |
| ATOM | 2526 | CD2 | TYR | A | 323 | 25.199 | 28.713 | 64.789 | 1.00 | 24.52 |
| ATOM | 2527 | CE1 | TYR | A | 323 | 26.530 | 27.974 | 67.157 | 1.00 | 22.56 |
| ATOM | 2528 | CE2 | TYR | A | 323 | 26.178 | 27.722 | 64.770 | 1.00 | 25.31 |
| ATOM | 2529 | CZ  | TYR | A | 323 | 26.846 | 27.370 | 65.944 | 1.00 | 29.19 |
| ATOM | 2530 | OH  | TYR | A | 323 | 27.823 | 26.434 | 65.895 | 1.00 | 27.51 |
| ATOM | 2531 | N   | LEU | A | 324 | 24.497 | 32.408 | 63.702 | 1.00 | 24.82 |
| ATOM | 2532 | CA  | LEU | A | 324 | 25.135 | 32.638 | 62.439 | 1.00 | 26.04 |
| ATOM | 2533 | C   | LEU | A | 324 | 25.832 | 33.952 | 62.417 | 1.00 | 30.92 |
| ATOM | 2534 | O   | LEU | A | 324 | 26.903 | 34.045 | 61.851 | 1.00 | 33.76 |
| ATOM | 2535 | CB  | LEU | A | 324 | 24.176 | 32.537 | 61.235 | 1.00 | 26.21 |
| ATOM | 2536 | CG  | LEU | A | 324 | 23.916 | 31.112 | 60.778 | 1.00 | 28.46 |
| ATOM | 2537 | CD1 | LEU | A | 324 | 22.752 | 31.109 | 59.791 | 1.00 | 28.95 |
| ATOM | 2538 | CD2 | LEU | A | 324 | 25.169 | 30.508 | 60.151 | 1.00 | 26.54 |
| ATOM | 2539 | N   | GLU | A | 325 | 25.234 | 34.976 | 63.033 | 1.00 | 27.04 |
| ATOM | 2540 | CA  | GLU | A | 325 | 25.870 | 36.303 | 63.064 | 1.00 | 22.88 |
| ATOM | 2541 | C   | GLU | A | 325 | 27.282 | 36.210 | 63.624 | 1.00 | 28.76 |
| ATOM | 2542 | O   | GLU | A | 325 | 28.250 | 36.722 | 63.026 | 1.00 | 26.24 |
| ATOM | 2543 | CB  | GLU | A | 325 | 25.016 | 37.365 | 63.759 | 1.00 | 22.01 |
| ATOM | 2544 | CG  | GLU | A | 325 | 25.827 | 38.411 | 64.524 | 1.00 | 41.55 |
| ATOM | 2545 | CD  | GLU | A | 325 | 25.035 | 39.040 | 65.646 | 1.00 | 72.11 |
| ATOM | 2546 | OE1 | GLU | A | 325 | 23.866 | 38.764 | 65.862 | 1.00 | 41.88 |
| ATOM | 2547 | OE2 | GLU | A | 325 | 25.719 | 39.922 | 66.350 | 1.00 | 67.15 |
| ATOM | 2548 | N   | ARG | A | 326 | 27.349 | 35.479 | 64.755 | 1.00 | 27.84 |
| ATOM | 2549 | CA  | ARG | A | 326 | 28.551 | 35.213 | 65.511 | 1.00 | 28.10 |
| ATOM | 2550 | C   | ARG | A | 326 | 29.604 | 34.457 | 64.771 | 1.00 | 30.90 |
| ATOM | 2551 | O   | ARG | A | 326 | 30.763 | 34.747 | 64.976 | 1.00 | 33.93 |
| ATOM | 2552 | CB  | ARG | A |     |        |        |        |      |       |



|      |      |     |     |   |     |        |        |        |      |        |
|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
| ATOM | 2571 | C   | ILE | A | 328 | 31.416 | 36.407 | 61.086 | 1.00 | 40.12  |
| ATOM | 2572 | O   | ILE | A | 328 | 32.451 | 36.615 | 60.465 | 1.00 | 40.81  |
| ATOM | 2573 | CB  | ILE | A | 328 | 29.175 | 36.379 | 59.998 | 1.00 | 32.94  |
| ATOM | 2574 | CG1 | ILE | A | 328 | 28.220 | 35.570 | 59.114 | 1.00 | 29.53  |
| ATOM | 2575 | CG2 | ILE | A | 328 | 29.694 | 37.591 | 59.201 | 1.00 | 30.91  |
| ATOM | 2576 | CD1 | ILE | A | 328 | 27.119 | 36.463 | 58.535 | 1.00 | 32.98  |
| ATOM | 2577 | N   | CYS | A | 329 | 31.179 | 36.948 | 62.266 | 1.00 | 37.88  |
| ATOM | 2578 | CA  | CYS | A | 329 | 32.170 | 37.810 | 62.851 | 1.00 | 39.54  |
| ATOM | 2579 | C   | CYS | A | 329 | 33.475 | 37.092 | 63.157 | 1.00 | 40.19  |
| ATOM | 2580 | O   | CYS | A | 329 | 34.567 | 37.642 | 62.971 | 1.00 | 38.44  |
| ATOM | 2581 | CB  | CYS | A | 329 | 31.607 | 38.509 | 64.083 | 1.00 | 42.63  |
| ATOM | 2582 | SG  | CYS | A | 329 | 30.241 | 39.595 | 63.619 | 1.00 | 48.14  |
| ATOM | 2583 | N   | GLY | A | 330 | 33.332 | 35.852 | 63.632 | 1.00 | 34.74  |
| ATOM | 2584 | CA  | GLY | A | 330 | 34.471 | 35.030 | 63.980 | 1.00 | 35.20  |
| ATOM | 2585 | C   | GLY | A | 330 | 35.359 | 34.854 | 62.778 | 1.00 | 43.66  |
| ATOM | 2586 | O   | GLY | A | 330 | 36.581 | 34.857 | 62.891 | 1.00 | 46.79  |
| ATOM | 2587 | N   | ARG | A | 331 | 34.709 | 34.725 | 61.622 | 1.00 | 34.99  |
| ATOM | 2588 | CA  | ARG | A | 331 | 35.416 | 34.562 | 60.392 | 1.00 | 33.19  |
| ATOM | 2589 | C   | ARG | A | 331 | 36.086 | 35.863 | 60.017 | 1.00 | 40.63  |
| ATOM | 2590 | O   | ARG | A | 331 | 37.238 | 35.914 | 59.586 | 1.00 | 44.40  |
| ATOM | 2591 | CB  | ARG | A | 331 | 34.494 | 34.101 | 59.269 | 1.00 | 31.29  |
| ATOM | 2592 | CG  | ARG | A | 331 | 33.987 | 32.685 | 59.450 | 1.00 | 47.66  |
| ATOM | 2593 | CD  | ARG | A | 331 | 34.812 | 31.722 | 58.622 | 1.00 | 70.36  |
| ATOM | 2594 | NE  | ARG | A | 331 | 34.461 | 31.851 | 57.221 | 1.00 | 80.25  |
| ATOM | 2595 | CZ  | ARG | A | 331 | 33.615 | 31.023 | 56.628 | 1.00 | 100.00 |
| ATOM | 2596 | NH1 | ARG | A | 331 | 33.055 | 29.999 | 57.279 | 1.00 | 79.12  |
| ATOM | 2597 | NH2 | ARG | A | 331 | 33.334 | 31.216 | 55.341 | 1.00 | 89.33  |
| ATOM | 2598 | N   | LEU | A | 332 | 35.342 | 36.926 | 60.172 | 1.00 | 32.14  |
| ATOM | 2599 | CA  | LEU | A | 332 | 35.885 | 38.198 | 59.820 | 1.00 | 30.02  |
| ATOM | 2600 | C   | LEU | A | 332 | 37.013 | 38.612 | 60.761 | 1.00 | 40.33  |
| ATOM | 2601 | O   | LEU | A | 332 | 38.084 | 38.972 | 60.286 | 1.00 | 40.10  |
| ATOM | 2602 | CB  | LEU | A | 332 | 34.772 | 39.262 | 59.822 | 1.00 | 28.20  |
| ATOM | 2603 | CG  | LEU | A | 332 | 34.451 | 39.896 | 58.469 | 1.00 | 28.82  |
| ATOM | 2604 | CD1 | LEU | A | 332 | 35.007 | 39.063 | 57.341 | 1.00 | 23.73  |
| ATOM | 2605 | CD2 | LEU | A | 332 | 32.947 | 40.114 | 58.306 | 1.00 | 29.76  |
| ATOM | 2606 | N   | PHE | A | 333 | 36.744 | 38.557 | 62.091 | 1.00 | 37.69  |
| ATOM | 2607 | CA  | PHE | A | 333 | 37.657 | 38.997 | 63.143 | 1.00 | 34.12  |
| ATOM | 2608 | C   | PHE | A | 333 | 38.251 | 37.956 | 64.035 | 1.00 | 37.99  |
| ATOM | 2609 | O   | PHE | A | 333 | 39.015 | 38.293 | 64.925 | 1.00 | 41.67  |
| ATOM | 2610 | CB  | PHE | A | 333 | 36.970 | 40.058 | 64.024 | 1.00 | 35.62  |
| ATOM | 2611 | CG  | PHE | A | 333 | 36.209 | 41.003 | 63.138 | 1.00 | 39.09  |
| ATOM | 2612 | CD1 | PHE | A | 333 | 36.887 | 41.923 | 62.332 | 1.00 | 43.22  |
| ATOM | 2613 | CD2 | PHE | A | 333 | 34.818 | 40     |        |      |        |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 2632 | C   | LYS | A | 336 | 37.445 | 35.726 | 70.169 | 1.00 | 35.32 |
| ATOM | 2633 | O   | LYS | A | 336 | 36.908 | 36.004 | 71.233 | 1.00 | 38.14 |
| ATOM | 2634 | CB  | LYS | A | 336 | 39.820 | 35.199 | 70.421 | 1.00 | 25.45 |
| ATOM | 2635 | CG  | LYS | A | 336 | 40.871 | 34.188 | 70.825 | 1.00 | 25.43 |
| ATOM | 2636 | CD  | LYS | A | 336 | 42.207 | 34.846 | 71.189 | 1.00 | 47.10 |
| ATOM | 2637 | CE  | LYS | A | 336 | 43.325 | 34.600 | 70.172 | 1.00 | 68.74 |
| ATOM | 2638 | NZ  | LYS | A | 336 | 44.566 | 34.072 | 70.767 | 1.00 | 77.62 |
| ATOM | 2639 | N   | PHE | A | 337 | 37.174 | 36.364 | 69.029 | 1.00 | 31.52 |
| ATOM | 2640 | CA  | PHE | A | 337 | 36.186 | 37.442 | 68.967 | 1.00 | 29.34 |
| ATOM | 2641 | C   | PHE | A | 337 | 34.783 | 36.869 | 69.083 | 1.00 | 31.73 |
| ATOM | 2642 | O   | PHE | A | 337 | 33.908 | 37.424 | 69.742 | 1.00 | 35.53 |
| ATOM | 2643 | CB  | PHE | A | 337 | 36.304 | 38.336 | 67.709 | 1.00 | 30.04 |
| ATOM | 2644 | CG  | PHE | A | 337 | 35.435 | 39.589 | 67.747 | 1.00 | 35.16 |
| ATOM | 2645 | CD1 | PHE | A | 337 | 35.468 | 40.459 | 68.843 | 1.00 | 43.88 |
| ATOM | 2646 | CD2 | PHE | A | 337 | 34.550 | 39.893 | 66.709 | 1.00 | 40.16 |
| ATOM | 2647 | CE1 | PHE | A | 337 | 34.688 | 41.617 | 68.913 | 1.00 | 46.53 |
| ATOM | 2648 | CE2 | PHE | A | 337 | 33.753 | 41.040 | 66.760 | 1.00 | 45.62 |
| ATOM | 2649 | CZ  | PHE | A | 337 | 33.830 | 41.908 | 67.852 | 1.00 | 45.57 |
| ATOM | 2650 | N   | ARG | A | 338 | 34.566 | 35.733 | 68.452 | 1.00 | 25.52 |
| ATOM | 2651 | CA  | ARG | A | 338 | 33.266 | 35.119 | 68.508 | 1.00 | 25.23 |
| ATOM | 2652 | C   | ARG | A | 338 | 32.944 | 34.759 | 69.922 | 1.00 | 29.77 |
| ATOM | 2653 | O   | ARG | A | 338 | 31.854 | 35.025 | 70.415 | 1.00 | 31.81 |
| ATOM | 2654 | CB  | ARG | A | 338 | 33.186 | 33.920 | 67.606 | 1.00 | 24.04 |
| ATOM | 2655 | CG  | ARG | A | 338 | 31.839 | 33.228 | 67.623 | 1.00 | 21.31 |
| ATOM | 2656 | CD  | ARG | A | 338 | 31.807 | 32.086 | 66.599 | 1.00 | 30.62 |
| ATOM | 2657 | NE  | ARG | A | 338 | 32.518 | 30.892 | 67.040 | 1.00 | 29.87 |
| ATOM | 2658 | CZ  | ARG | A | 338 | 31.919 | 29.781 | 67.466 | 1.00 | 26.37 |
| ATOM | 2659 | NH1 | ARG | A | 338 | 30.616 | 29.687 | 67.518 | 1.00 | 20.26 |
| ATOM | 2660 | NH2 | ARG | A | 338 | 32.632 | 28.737 | 67.864 | 1.00 | 18.57 |
| ATOM | 2661 | N   | HIS | A | 339 | 33.934 | 34.190 | 70.577 | 1.00 | 25.88 |
| ATOM | 2662 | CA  | HIS | A | 339 | 33.813 | 33.797 | 71.982 | 1.00 | 25.59 |
| ATOM | 2663 | C   | HIS | A | 339 | 33.455 | 34.972 | 72.892 | 1.00 | 27.61 |
| ATOM | 2664 | O   | HIS | A | 339 | 32.615 | 34.912 | 73.793 | 1.00 | 25.27 |
| ATOM | 2665 | CB  | HIS | A | 339 | 35.065 | 33.045 | 72.462 | 1.00 | 25.06 |
| ATOM | 2666 | CG  | HIS | A | 339 | 34.923 | 31.587 | 72.155 | 1.00 | 28.13 |
| ATOM | 2667 | ND1 | HIS | A | 339 | 35.049 | 30.612 | 73.127 | 1.00 | 30.52 |
| ATOM | 2668 | CD2 | HIS | A | 339 | 34.586 | 30.970 | 70.981 | 1.00 | 30.89 |
| ATOM | 2669 | CE1 | HIS | A | 339 | 34.843 | 29.442 | 72.535 | 1.00 | 30.89 |
| ATOM | 2670 | NE2 | HIS | A | 339 | 34.546 | 29.616 | 71.245 | 1.00 | 31.36 |
| ATOM | 2671 | N   | PHE | A | 340 | 34.103 | 36.065 | 72.608 | 1.00 | 24.54 |
| ATOM | 2672 | CA  | PHE | A | 340 | 33.892 | 37.278 | 73.334 | 1.00 | 25.36 |
| ATOM | 2673 | C   | PHE | A | 340 | 32.452 | 37.762 | 73.216 | 1.00 | 32.47 |
| ATOM | 2674 | O   | PHE | A | 340 | 31.822 | 38.222 | 74.190 | 1.00 | 32.78 |
| ATOM | 2675 | CB  | PHE | A | 340 | 34.876 | 38.309 | 72.801 | 1.00 | 26.03 |
| ATOM | 2676 | CG  | PHE | A | 340 | 34.654 | 39.671 | 73.346 | 1.00 | 26.47 |
| ATOM | 2677 | CD1 | PHE | A | 340 | 35.238 | 40.047 | 74.559 | 1.00 | 24.59 |
| ATOM | 2678 | CD2 | PHE | A | 340 | 33.902 | 40.592 | 72.616 | 1.00 | 28.22 |
| ATOM | 2679 | CE1 | PHE | A | 340 | 35.063 | 41.330 | 75.072 | 1.00 | 21.58 |
| ATOM | 2680 | CE2 | PHE | A | 340 | 33.715 | 41.879 | 73.115 | 1.00 | 29.13 |
| ATOM | 2681 | CZ  | PHE | A | 340 | 34.280 | 42.225 | 74.345 | 1.00 | 25.28 |
| ATOM | 2682 | N   | ASN | A | 341 | 31.944 | 37.663 | 72.004 | 1.00 | 28.41 |
| ATOM | 2683 | CA  | ASN | A | 341 | 30.600 | 38.084 | 71.728 | 1.00 | 29.60 |
| ATOM | 2684 | C   | ASN | A | 341 | 29.665 | 37.110 | 72.379 | 1.00 | 38.52 |
| ATOM | 2685 | O   | ASN | A | 341 | 28.699 | 37.511 | 73.029 | 1.00 | 42.88 |
| ATOM | 2686 | CB  | ASN | A | 341 | 30.322 | 38.274 | 70.224 | 1.00 | 30.01 |
| ATOM | 2687 | CG  | ASN | A | 341 | 31.159 | 39.374 | 69.587 | 1.00 | 52.80 |
| ATOM | 2688 | OD1 | ASN | A | 341 | 31.528 | 39.284 | 68.404 | 1.00 | 60.88 |
| ATOM | 2689 | ND2 | ASN | A | 341 | 31.442 | 40.427 | 70.359 | 1.00 | 41.02 |
| ATOM | 2690 | N   | ALA | A | 342 | 29.994 | 35.826 | 72.239 | 1.00 | 28.24 |
| ATOM | 2691 | CA  | ALA | A | 342 | 29.195 | 34.800 | 72.877 | 1.00 | 26.95 |
| ATOM | 2692 | C   | ALA | A | 342 | 29.013 | 35.134 | 74.393 | 1.00 | 35.98 |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 2693 | O   | ALA | A | 342 | 27.877 | 35.261 | 74.897 | 1.00 | 35.09 |
| ATOM | 2694 | CB  | ALA | A | 342 | 29.837 | 33.422 | 72.671 | 1.00 | 25.45 |
| ATOM | 2695 | N   | LEU | A | 343 | 30.153 | 35.304 | 75.122 | 1.00 | 29.16 |
| ATOM | 2696 | CA  | LEU | A | 343 | 30.162 | 35.633 | 76.560 | 1.00 | 22.58 |
| ATOM | 2697 | C   | LEU | A | 343 | 29.310 | 36.854 | 76.831 | 1.00 | 27.48 |
| ATOM | 2698 | O   | LEU | A | 343 | 28.452 | 36.821 | 77.696 | 1.00 | 32.73 |
| ATOM | 2699 | CB  | LEU | A | 343 | 31.583 | 35.786 | 77.147 | 1.00 | 18.70 |
| ATOM | 2700 | CG  | LEU | A | 343 | 31.647 | 35.693 | 78.671 | 1.00 | 20.08 |
| ATOM | 2701 | CD1 | LEU | A | 343 | 30.842 | 34.510 | 79.204 | 1.00 | 17.76 |
| ATOM | 2702 | CD2 | LEU | A | 343 | 33.091 | 35.522 | 79.111 | 1.00 | 21.94 |
| ATOM | 2703 | N   | GLY | A | 344 | 29.512 | 37.936 | 76.080 | 1.00 | 22.60 |
| ATOM | 2704 | CA  | GLY | A | 344 | 28.670 | 39.146 | 76.278 | 1.00 | 24.15 |
| ATOM | 2705 | C   | GLY | A | 344 | 27.157 | 38.824 | 76.136 | 1.00 | 31.38 |
| ATOM | 2706 | O   | GLY | A | 344 | 26.339 | 39.260 | 76.943 | 1.00 | 32.44 |
| ATOM | 2707 | N   | GLY | A | 345 | 26.806 | 38.017 | 75.094 | 1.00 | 22.79 |
| ATOM | 2708 | CA  | GLY | A | 345 | 25.451 | 37.587 | 74.801 | 1.00 | 19.88 |
| ATOM | 2709 | C   | GLY | A | 345 | 24.787 | 36.994 | 76.034 | 1.00 | 28.37 |
| ATOM | 2710 | O   | GLY | A | 345 | 23.632 | 37.294 | 76.325 | 1.00 | 27.56 |
| ATOM | 2711 | N   | TRP | A | 346 | 25.547 | 36.153 | 76.765 | 1.00 | 25.41 |
| ATOM | 2712 | CA  | TRP | A | 346 | 25.082 | 35.520 | 77.994 | 1.00 | 23.90 |
| ATOM | 2713 | C   | TRP | A | 346 | 24.825 | 36.541 | 79.071 | 1.00 | 31.54 |
| ATOM | 2714 | O   | TRP | A | 346 | 23.957 | 36.379 | 79.924 | 1.00 | 29.57 |
| ATOM | 2715 | CB  | TRP | A | 346 | 26.122 | 34.556 | 78.562 | 1.00 | 21.53 |
| ATOM | 2716 | CG  | TRP | A | 346 | 25.680 | 33.880 | 79.837 | 1.00 | 21.92 |
| ATOM | 2717 | CD1 | TRP | A | 346 | 25.933 | 34.335 | 81.079 | 1.00 | 24.36 |
| ATOM | 2718 | CD2 | TRP | A | 346 | 25.004 | 32.597 | 80.010 | 1.00 | 20.97 |
| ATOM | 2719 | NE1 | TRP | A | 346 | 25.450 | 33.453 | 82.008 | 1.00 | 23.95 |
| ATOM | 2720 | CE2 | TRP | A | 346 | 24.859 | 32.388 | 81.391 | 1.00 | 24.13 |
| ATOM | 2721 | CE3 | TRP | A | 346 | 24.488 | 31.611 | 79.144 | 1.00 | 21.46 |
| ATOM | 2722 | CZ2 | TRP | A | 346 | 24.225 | 31.244 | 81.921 | 1.00 | 22.89 |
| ATOM | 2723 | CZ3 | TRP | A | 346 | 23.872 | 30.477 | 79.662 | 1.00 | 22.03 |
| ATOM | 2724 | CH2 | TRP | A | 346 | 23.747 | 30.286 | 81.046 | 1.00 | 21.87 |
| ATOM | 2725 | N   | GLY | A | 347 | 25.627 | 37.593 | 79.039 | 1.00 | 29.66 |
| ATOM | 2726 | CA  | GLY | A | 347 | 25.465 | 38.625 | 80.042 | 1.00 | 29.03 |
| ATOM | 2727 | C   | GLY | A | 347 | 24.156 | 39.333 | 79.844 | 1.00 | 33.01 |
| ATOM | 2728 | O   | GLY | A | 347 | 23.491 | 39.647 | 80.799 | 1.00 | 34.17 |
| ATOM | 2729 | N   | GLU | A | 348 | 23.797 | 39.574 | 78.581 | 1.00 | 30.57 |
| ATOM | 2730 | CA  | GLU | A | 348 | 22.535 | 40.220 | 78.250 | 1.00 | 29.17 |
| ATOM | 2731 | C   | GLU | A | 348 | 21.423 | 39.282 | 78.664 | 1.00 | 31.25 |
| ATOM | 2732 | O   | GLU | A | 348 | 20.373 | 39.663 | 79.142 | 1.00 | 33.71 |
| ATOM | 2733 | CB  | GLU | A | 348 | 22.432 | 40.606 | 76.757 | 1.00 | 30.33 |
| ATOM | 2734 | CG  | GLU | A | 348 | 23.432 | 41.715 | 76.336 | 1.00 | 49.41 |
| ATOM | 2735 | CD  | GLU |   |     |        |        |        |      |       |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 2754 | NE2 | GLN | A | 350 | 25.588 | 37.727 | 83.127 | 1.00 | 36.58 |
| ATOM | 2755 | N   | ASN | A | 351 | 20.838 | 39.696 | 82.201 | 1.00 | 22.64 |
| ATOM | 2756 | CA  | ASN | A | 351 | 20.163 | 40.960 | 82.273 | 1.00 | 26.10 |
| ATOM | 2757 | C   | ASN | A | 351 | 18.661 | 40.780 | 82.083 | 1.00 | 37.49 |
| ATOM | 2758 | O   | ASN | A | 351 | 17.890 | 41.098 | 82.977 | 1.00 | 41.41 |
| ATOM | 2759 | CB  | ASN | A | 351 | 20.769 | 42.021 | 81.341 | 1.00 | 20.74 |
| ATOM | 2760 | CG  | ASN | A | 351 | 22.118 | 42.477 | 81.847 | 1.00 | 23.25 |
| ATOM | 2761 | OD1 | ASN | A | 351 | 22.692 | 41.875 | 82.771 | 1.00 | 26.88 |
| ATOM | 2762 | ND2 | ASN | A | 351 | 22.644 | 43.530 | 81.247 | 1.00 | 32.93 |
| ATOM | 2763 | N   | SER | A | 352 | 18.228 | 40.252 | 80.938 | 1.00 | 32.84 |
| ATOM | 2764 | CA  | SER | A | 352 | 16.784 | 40.041 | 80.715 | 1.00 | 34.27 |
| ATOM | 2765 | C   | SER | A | 352 | 16.107 | 39.135 | 81.784 | 1.00 | 31.72 |
| ATOM | 2766 | O   | SER | A | 352 | 14.927 | 39.266 | 82.189 | 1.00 | 28.64 |
| ATOM | 2767 | CB  | SER | A | 352 | 16.503 | 39.531 | 79.301 | 1.00 | 42.57 |
| ATOM | 2768 | OG  | SER | A | 352 | 17.506 | 39.979 | 78.407 | 1.00 | 49.17 |
| ATOM | 2769 | N   | VAL | A | 353 | 16.874 | 38.188 | 82.247 | 1.00 | 21.90 |
| ATOM | 2770 | CA  | VAL | A | 353 | 16.322 | 37.351 | 83.234 | 1.00 | 22.13 |
| ATOM | 2771 | C   | VAL | A | 353 | 16.068 | 38.122 | 84.516 | 1.00 | 36.22 |
| ATOM | 2772 | O   | VAL | A | 353 | 14.958 | 38.076 | 85.052 | 1.00 | 37.69 |
| ATOM | 2773 | CB  | VAL | A | 353 | 17.137 | 36.070 | 83.419 | 1.00 | 20.84 |
| ATOM | 2774 | CG1 | VAL | A | 353 | 16.632 | 35.256 | 84.634 | 1.00 | 15.06 |
| ATOM | 2775 | CG2 | VAL | A | 353 | 16.968 | 35.284 | 82.105 | 1.00 | 20.93 |
| ATOM | 2776 | N   | LYS | A | 354 | 17.086 | 38.847 | 85.002 | 1.00 | 30.67 |
| ATOM | 2777 | CA  | LYS | A | 354 | 16.880 | 39.587 | 86.221 | 1.00 | 31.71 |
| ATOM | 2778 | C   | LYS | A | 354 | 15.660 | 40.474 | 86.098 | 1.00 | 36.17 |
| ATOM | 2779 | O   | LYS | A | 354 | 14.808 | 40.582 | 86.980 | 1.00 | 35.80 |
| ATOM | 2780 | CB  | LYS | A | 354 | 18.099 | 40.396 | 86.624 | 1.00 | 35.28 |
| ATOM | 2781 | CG  | LYS | A | 354 | 17.841 | 41.303 | 87.818 | 1.00 | 51.51 |
| ATOM | 2782 | CD  | LYS | A | 354 | 19.038 | 41.405 | 88.749 | 1.00 | 60.46 |
| ATOM | 2783 | CE  | LYS | A | 354 | 19.198 | 42.780 | 89.383 | 1.00 | 50.09 |
| ATOM | 2784 | NZ  | LYS | A | 354 | 20.596 | 43.133 | 89.657 | 1.00 | 63.77 |
| ATOM | 2785 | N   | THR | A | 355 | 15.608 | 41.108 | 84.962 | 1.00 | 32.63 |
| ATOM | 2786 | CA  | THR | A | 355 | 14.562 | 42.025 | 84.610 | 1.00 | 34.03 |
| ATOM | 2787 | C   | THR | A | 355 | 13.129 | 41.422 | 84.578 | 1.00 | 42.11 |
| ATOM | 2788 | O   | THR | A | 355 | 12.216 | 42.006 | 85.154 | 1.00 | 40.96 |
| ATOM | 2789 | CB  | THR | A | 355 | 14.974 | 42.736 | 83.308 | 1.00 | 41.11 |
| ATOM | 2790 | OG1 | THR | A | 355 | 16.071 | 43.615 | 83.542 | 1.00 | 29.85 |
| ATOM | 2791 | CG2 | THR | A | 355 | 13.798 | 43.438 | 82.656 | 1.00 | 45.50 |
| ATOM | 2792 | N   | PHE | A | 356 | 12.895 | 40.273 | 83.908 | 1.00 | 33.89 |
| ATOM | 2793 | CA  | PHE | A | 356 | 11.556 | 39.729 | 83.860 | 1.00 | 29.29 |
| ATOM | 2794 | C   | PHE | A | 356 | 11.209 | 39.070 | 85.147 | 1.00 | 31.93 |
| ATOM | 2795 | O   | PHE | A | 356 | 10.089 | 39.152 | 85.642 | 1.00 | 33.85 |
| ATOM | 2796 | CB  | PHE | A | 356 | 11.460 | 38.645 | 82.785 | 1.00 | 33.30 |
| ATOM | 2797 | CG  | PHE | A | 356 | 11.187 | 39.196 | 81.416 | 1.00 | 36.54 |
| ATOM | 2798 | CD1 | PHE | A | 356 | 10.106 | 40.054 | 81.224 | 1.00 | 42.38 |
| ATOM | 2799 | CD2 | PHE | A | 356 | 11.985 | 38.858 | 80.320 | 1.00 | 38.62 |
| ATOM | 2800 | CE1 | PHE | A | 356 | 9.831  | 40.596 | 79.968 | 1.00 | 44.75 |
| ATOM | 2801 | CE2 | PHE | A | 356 | 11.723 | 39.384 | 79.055 | 1.00 | 43.46 |
| ATOM | 2802 | CZ  | PHE | A | 356 | 10.649 | 40.261 | 78.890 | 1.00 | 43.86 |
| ATOM | 2803 | N   | GLY | A | 357 | 12.212 | 38.386 | 85.661 | 1.00 | 30.41 |
| ATOM | 2804 | CA  | GLY | A | 357 | 12.152 | 37.564 | 86.864 | 1.00 | 29.17 |
| ATOM | 2805 | C   | GLY | A | 357 | 12.446 | 36.100 | 86.438 | 1.00 | 28.92 |
| ATOM | 2806 | O   | GLY | A | 357 | 12.008 | 35.642 | 85.372 | 1.00 | 27.33 |
| ATOM | 2807 | N   | GLU | A | 358 | 13.211 | 35.382 | 87.243 | 1.00 | 21.27 |
| ATOM | 2808 | CA  | GLU | A | 358 | 13.590 | 34.040 | 86.898 | 1.00 | 23.10 |
| ATOM | 2809 | C   | GLU | A | 358 | 12.424 | 33.104 | 86.747 | 1.00 | 31.53 |
| ATOM | 2810 | O   | GLU | A | 358 | 12.581 | 31.972 | 86.294 | 1.00 | 30.92 |
| ATOM | 2811 | CB  | GLU | A | 358 | 14.596 | 33.473 | 87.880 | 1.00 | 25.36 |
| ATOM | 2812 | CG  | GLU | A | 358 | 14.011 | 33.436 | 89.301 | 1.00 | 38.73 |
| ATOM | 2813 | CD  | GLU | A | 358 | 15.011 | 33.037 | 90.345 | 1.00 | 56.34 |
| ATOM | 2814 | OE1 | GLU | A | 358 | 16.026 | 32.446 | 90.071 | 1.00 | 50.55 |



004224.00 : 022600

|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 2815 | OE2 | GLU | A | 358 | 14.678 | 33.403 | 91.564 | 1.00 | 75.65 |
| ATOM | 2816 | N   | THR | A | 359 | 11.246 | 33.542 | 87.139 | 1.00 | 27.87 |
| ATOM | 2817 | CA  | THR | A | 359 | 10.154 | 32.625 | 86.970 | 1.00 | 25.66 |
| ATOM | 2818 | C   | THR | A | 359 | 9.236  | 33.152 | 85.906 | 1.00 | 25.96 |
| ATOM | 2819 | O   | THR | A | 359 | 8.247  | 32.528 | 85.533 | 1.00 | 25.58 |
| ATOM | 2820 | CB  | THR | A | 359 | 9.423  | 32.341 | 88.253 | 1.00 | 25.00 |
| ATOM | 2821 | OG1 | THR | A | 359 | 8.908  | 33.565 | 88.692 | 1.00 | 33.10 |
| ATOM | 2822 | CG2 | THR | A | 359 | 10.406 | 31.785 | 89.273 | 1.00 | 14.43 |
| ATOM | 2823 | N   | HIS | A | 360 | 9.602  | 34.310 | 85.407 | 1.00 | 20.75 |
| ATOM | 2824 | CA  | HIS | A | 360 | 8.837  | 34.902 | 84.363 | 1.00 | 22.77 |
| ATOM | 2825 | C   | HIS | A | 360 | 8.823  | 34.034 | 83.130 | 1.00 | 35.30 |
| ATOM | 2826 | O   | HIS | A | 360 | 9.858  | 33.611 | 82.620 | 1.00 | 37.42 |
| ATOM | 2827 | CB  | HIS | A | 360 | 9.294  | 36.291 | 83.982 | 1.00 | 23.18 |
| ATOM | 2828 | CG  | HIS | A | 360 | 8.207  | 36.908 | 83.219 | 1.00 | 27.05 |
| ATOM | 2829 | ND1 | HIS | A | 360 | 7.532  | 38.009 | 83.691 | 1.00 | 29.34 |
| ATOM | 2830 | CD2 | HIS | A | 360 | 7.651  | 36.545 | 82.059 | 1.00 | 29.91 |
| ATOM | 2831 | CE1 | HIS | A | 360 | 6.596  | 38.315 | 82.806 | 1.00 | 27.94 |
| ATOM | 2832 | NE2 | HIS | A | 360 | 6.651  | 37.440 | 81.812 | 1.00 | 29.60 |
| ATOM | 2833 | N   | PRO | A | 361 | 7.606  | 33.817 | 82.666 | 1.00 | 32.40 |
| ATOM | 2834 | CA  | PRO | A | 361 | 7.301  | 32.999 | 81.519 | 1.00 | 29.46 |
| ATOM | 2835 | C   | PRO | A | 361 | 7.862  | 33.478 | 80.224 | 1.00 | 30.59 |
| ATOM | 2836 | O   | PRO | A | 361 | 7.907  | 32.737 | 79.248 | 1.00 | 33.00 |
| ATOM | 2837 | CB  | PRO | A | 361 | 5.770  | 32.963 | 81.478 | 1.00 | 30.74 |
| ATOM | 2838 | CG  | PRO | A | 361 | 5.311  | 33.172 | 82.927 | 1.00 | 34.96 |
| ATOM | 2839 | CD  | PRO | A | 361 | 6.463  | 33.869 | 83.627 | 1.00 | 31.82 |
| ATOM | 2840 | N   | PHE | A | 362 | 8.289  | 34.712 | 80.179 | 1.00 | 26.32 |
| ATOM | 2841 | CA  | PHE | A | 362 | 8.823  | 35.173 | 78.933 | 1.00 | 25.68 |
| ATOM | 2842 | C   | PHE | A | 362 | 10.261 | 34.781 | 78.829 | 1.00 | 29.73 |
| ATOM | 2843 | O   | PHE | A | 362 | 10.906 | 35.131 | 77.870 | 1.00 | 32.02 |
| ATOM | 2844 | CB  | PHE | A | 362 | 8.643  | 36.677 | 78.723 | 1.00 | 28.12 |
| ATOM | 2845 | CG  | PHE | A | 362 | 7.194  | 37.105 | 78.629 | 1.00 | 30.03 |
| ATOM | 2846 | CD1 | PHE | A | 362 | 6.204  | 36.276 | 78.098 | 1.00 | 30.92 |
| ATOM | 2847 | CD2 | PHE | A | 362 | 6.804  | 38.372 | 79.051 | 1.00 | 32.04 |
| ATOM | 2848 | CE1 | PHE | A | 362 | 4.864  | 36.655 | 77.998 | 1.00 | 26.59 |
| ATOM | 2849 | CE2 | PHE | A | 362 | 5.470  | 38.773 | 78.952 | 1.00 | 32.40 |
| ATOM | 2850 | CZ  | PHE | A | 362 | 4.495  | 37.920 | 78.435 | 1.00 | 26.37 |
| ATOM | 2851 | N   | THR | A | 363 | 10.730 | 34.049 | 79.843 | 1.00 | 27.22 |
| ATOM | 2852 | CA  | THR | A | 363 | 12.102 | 33.575 | 79.943 | 1.00 | 27.52 |
| ATOM | 2853 | C   | THR | A | 363 | 12.251 | 32.132 | 79.504 | 1.00 | 29.28 |
| ATOM | 2854 | O   | THR | A | 363 | 13.331 | 31.560 | 79.524 | 1.00 | 29.42 |
| ATOM | 2855 | CB  | THR | A | 363 | 12.697 | 33.777 | 81.360 | 1.00 | 31.67 |
| ATOM | 2856 | OG1 | THR | A | 363 | 12.279 | 32.745 | 82.218 | 1.00 | 26.17 |
| ATOM | 2857 | CG2 | THR | A | 363 | 12.278 | 35.118 | 81.930 | 1.00 | 31.62 |
| ATOM | 2858 | N   | LYS | A | 364 | 11.148 | 31.530 | 79.113 | 1.00 | 23.08 |
| ATOM | 2859 | CA  | LYS | A | 364 | 11.174 | 30.160 | 78.664 | 1.00 | 20.50 |
| ATOM | 2860 | C   | LYS | A | 364 | 11.556 | 30.270 | 77.217 | 1.00 | 28.83 |
| ATOM | 2861 | O   | LYS | A | 364 | 11.139 | 31.239 | 76.570 | 1.00 | 29.80 |
| ATOM | 2862 | CB  | LYS | A | 364 | 9.766  | 29.584 | 78.667 | 1.00 | 23.55 |
| ATOM | 2863 | CG  | LYS | A | 364 | 9.252  | 29.134 | 80.022 | 1.00 | 40.85 |
| ATOM | 2864 | CD  | LYS | A | 364 | 7.761  | 29.369 | 80.162 | 1.00 | 44.83 |
| ATOM | 2865 | CE  | LYS | A | 364 | 7.131  | 28.492 | 81.224 | 1.00 | 66.38 |
| ATOM | 2866 | NZ  | LYS | A | 364 | 6.063  | 27.638 | 80.691 | 1.00 | 91.70 |
| ATOM | 2867 | N   | LEU | A | 365 | 12.332 | 29.328 | 76.698 | 1.00 | 23.57 |
| ATOM | 2868 | CA  | LEU | A | 365 | 12.699 | 29.420 | 75.312 | 1.00 | 23.95 |
| ATOM | 2869 | C   | LEU | A | 365 | 11.414 | 29.419 | 74.445 | 1.00 | 35.57 |
| ATOM | 2870 | O   | LEU | A | 365 | 11.166 | 30.369 | 73.708 | 1.00 | 34.58 |
| ATOM | 2871 | CB  | LEU | A | 365 | 13.702 | 28.303 | 75.021 | 1.00 | 25.08 |
| ATOM | 2872 | CG  | LEU | A | 365 | 14.456 | 28.372 | 73.702 | 1.00 | 31.15 |
| ATOM | 2873 | CD1 | LEU | A | 365 | 14.987 | 29.778 | 73.466 | 1.00 | 33.16 |
| ATOM | 2874 | CD2 | LEU | A | 365 | 15.609 | 27.353 | 73.781 | 1.00 | 30.62 |
| ATOM | 2875 | N   | VAL | A | 366 | 10.572 | 28.360 | 74.564 | 1.00 | 35.62 |



|      |      |     |           |        |        |        |      |       |
|------|------|-----|-----------|--------|--------|--------|------|-------|
| ATOM | 2876 | CA  | VAL A 366 | 9.294  | 28.232 | 73.840 | 1.00 | 32.10 |
| ATOM | 2877 | C   | VAL A 366 | 8.211  | 28.911 | 74.694 | 1.00 | 33.14 |
| ATOM | 2878 | O   | VAL A 366 | 7.982  | 28.470 | 75.808 | 1.00 | 34.20 |
| ATOM | 2879 | CB  | VAL A 366 | 8.936  | 26.739 | 73.568 | 1.00 | 34.73 |
| ATOM | 2880 | CG1 | VAL A 366 | 7.558  | 26.605 | 72.933 | 1.00 | 34.88 |
| ATOM | 2881 | CG2 | VAL A 366 | 9.922  | 26.012 | 72.649 | 1.00 | 32.65 |
| ATOM | 2882 | N   | VAL A 367 | 7.562  | 29.990 | 74.211 | 1.00 | 28.76 |
| ATOM | 2883 | CA  | VAL A 367 | 6.532  | 30.700 | 74.987 | 1.00 | 28.27 |
| ATOM | 2884 | C   | VAL A 367 | 5.161  | 30.613 | 74.420 | 1.00 | 30.62 |
| ATOM | 2885 | O   | VAL A 367 | 4.994  | 30.509 | 73.235 | 1.00 | 34.30 |
| ATOM | 2886 | CB  | VAL A 367 | 6.773  | 32.185 | 75.061 | 1.00 | 33.45 |
| ATOM | 2887 | CG1 | VAL A 367 | 8.178  | 32.478 | 75.565 | 1.00 | 33.03 |
| ATOM | 2888 | CG2 | VAL A 367 | 6.498  | 32.804 | 73.693 | 1.00 | 33.18 |
| ATOM | 2889 | N   | ASP A 368 | 4.168  | 30.722 | 75.290 | 1.00 | 29.27 |
| ATOM | 2890 | CA  | ASP A 368 | 2.764  | 30.771 | 74.984 | 1.00 | 27.67 |
| ATOM | 2891 | C   | ASP A 368 | 2.315  | 32.207 | 74.862 | 1.00 | 26.94 |
| ATOM | 2892 | O   | ASP A 368 | 2.283  | 32.975 | 75.830 | 1.00 | 23.11 |
| ATOM | 2893 | CB  | ASP A 368 | 1.990  | 30.073 | 76.100 | 1.00 | 26.80 |
| ATOM | 2894 | CG  | ASP A 368 | 0.572  | 29.781 | 75.613 | 1.00 | 37.90 |
| ATOM | 2895 | OD1 | ASP A 368 | 0.276  | 30.123 | 74.481 | 1.00 | 38.93 |
| ATOM | 2896 | OD2 | ASP A 368 | -0.215 | 29.217 | 76.380 | 1.00 | 38.59 |
| ATOM | 2897 | N   | LEU A 369 | 2.027  | 32.588 | 73.622 | 1.00 | 26.55 |
| ATOM | 2898 | CA  | LEU A 369 | 1.643  | 33.953 | 73.373 | 1.00 | 27.39 |
| ATOM | 2899 | C   | LEU A 369 | 0.138  | 34.105 | 73.301 | 1.00 | 30.74 |
| ATOM | 2900 | O   | LEU A 369 | -0.372 | 34.979 | 72.648 | 1.00 | 30.68 |
| ATOM | 2901 | CB  | LEU A 369 | 2.281  | 34.395 | 72.064 | 1.00 | 26.06 |
| ATOM | 2902 | CG  | LEU A 369 | 3.759  | 34.760 | 72.229 | 1.00 | 26.80 |
| ATOM | 2903 | CD1 | LEU A 369 | 4.343  | 35.415 | 70.994 | 1.00 | 24.30 |
| ATOM | 2904 | CD2 | LEU A 369 | 4.014  | 35.728 | 73.384 | 1.00 | 21.81 |
| ATOM | 2905 | N   | THR A 370 | -0.577 | 33.154 | 73.953 | 1.00 | 30.26 |
| ATOM | 2906 | CA  | THR A 370 | -2.022 | 33.306 | 74.093 | 1.00 | 31.38 |
| ATOM | 2907 | C   | THR A 370 | -2.355 | 34.519 | 74.941 | 1.00 | 38.62 |
| ATOM | 2908 | O   | THR A 370 | -1.821 | 34.714 | 76.027 | 1.00 | 38.84 |
| ATOM | 2909 | CB  | THR A 370 | -2.601 | 32.056 | 74.750 | 1.00 | 34.04 |
| ATOM | 2910 | OG1 | THR A 370 | -2.472 | 30.949 | 73.873 | 1.00 | 29.99 |
| ATOM | 2911 | CG2 | THR A 370 | -4.091 | 32.266 | 75.052 | 1.00 | 26.40 |
| ATOM | 2912 | N   | ASP A 371 | -3.173 | 35.387 | 74.363 | 1.00 | 37.89 |
| ATOM | 2913 | CA  | ASP A 371 | -3.641 | 36.612 | 75.012 | 1.00 | 37.85 |
| ATOM | 2914 | C   | ASP A 371 | -2.557 | 37.636 | 75.255 | 1.00 | 40.92 |
| ATOM | 2915 | O   | ASP A 371 | -2.784 | 38.625 | 75.933 | 1.00 | 41.63 |
| ATOM | 2916 | CB  | ASP A 371 | -4.519 | 36.375 | 76.245 | 1.00 | 39.88 |
| ATOM | 2917 | CG  | ASP A 371 | -5.805 | 35.733 | 75.798 | 1.00 | 51.30 |
| ATOM | 2918 | OD1 | ASP A 371 | -6.373 | 36.072 | 74.761 | 1.00 | 50.39 |
| ATOM | 2919 | OD2 | ASP A 371 | -6.206 | 34.754 | 76.583 | 1.00 | 48.61 |
| ATOM | 2920 | N   | ILE A 372 | -1.387 | 37.398 | 74.664 | 1.00 | 36.37 |
| ATOM | 2921 | CA  | ILE A 372 | -0.259 | 38.283 | 74.817 | 1.00 | 34.61 |
| ATOM | 2922 | C   | ILE A 372 | 0.203  | 39.018 | 73.555 | 1.00 | 35.46 |
|      |      |     |           |        |        |        |      |       |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 2937 | CA  | PRO | A | 374 | 4.123  | 39.943 | 71.132 | 1.00 | 28.52 |
| ATOM | 2938 | C   | PRO | A | 374 | 5.029  | 41.090 | 71.506 | 1.00 | 32.54 |
| ATOM | 2939 | O   | PRO | A | 374 | 6.019  | 40.905 | 72.217 | 1.00 | 29.62 |
| ATOM | 2940 | CB  | PRO | A | 374 | 4.390  | 39.421 | 69.714 | 1.00 | 28.88 |
| ATOM | 2941 | CG  | PRO | A | 374 | 3.028  | 39.278 | 69.032 | 1.00 | 32.27 |
| ATOM | 2942 | CD  | PRO | A | 374 | 1.966  | 39.786 | 70.008 | 1.00 | 28.84 |
| ATOM | 2943 | N   | ASP | A | 375 | 4.660  | 42.257 | 70.981 | 1.00 | 26.85 |
| ATOM | 2944 | CA  | ASP | A | 375 | 5.357  | 43.511 | 71.154 | 1.00 | 24.25 |
| ATOM | 2945 | C   | ASP | A | 375 | 5.695  | 43.783 | 72.628 | 1.00 | 33.10 |
| ATOM | 2946 | O   | ASP | A | 375 | 6.648  | 44.494 | 72.988 | 1.00 | 30.67 |
| ATOM | 2947 | CB  | ASP | A | 375 | 4.507  | 44.617 | 70.509 | 1.00 | 24.46 |
| ATOM | 2948 | CG  | ASP | A | 375 | 4.753  | 44.836 | 69.033 | 1.00 | 30.08 |
| ATOM | 2949 | OD1 | ASP | A | 375 | 5.703  | 44.393 | 68.411 | 1.00 | 33.47 |
| ATOM | 2950 | OD2 | ASP | A | 375 | 3.852  | 45.609 | 68.491 | 1.00 | 38.41 |
| ATOM | 2951 | N   | VAL | A | 376 | 4.885  | 43.161 | 73.477 | 1.00 | 30.21 |
| ATOM | 2952 | CA  | VAL | A | 376 | 5.001  | 43.232 | 74.904 | 1.00 | 25.40 |
| ATOM | 2953 | C   | VAL | A | 376 | 5.879  | 42.106 | 75.431 | 1.00 | 37.27 |
| ATOM | 2954 | O   | VAL | A | 376 | 6.599  | 42.299 | 76.394 | 1.00 | 42.46 |
| ATOM | 2955 | CB  | VAL | A | 376 | 3.638  | 43.099 | 75.550 | 1.00 | 22.48 |
| ATOM | 2956 | CG1 | VAL | A | 376 | 3.799  | 42.533 | 76.975 | 1.00 | 21.25 |
| ATOM | 2957 | CG2 | VAL | A | 376 | 2.926  | 44.440 | 75.547 | 1.00 | 18.29 |
| ATOM | 2958 | N   | ALA | A | 377 | 5.811  | 40.905 | 74.831 | 1.00 | 30.48 |
| ATOM | 2959 | CA  | ALA | A | 377 | 6.671  | 39.793 | 75.288 | 1.00 | 27.04 |
| ATOM | 2960 | C   | ALA | A | 377 | 8.149  | 39.911 | 74.797 | 1.00 | 28.15 |
| ATOM | 2961 | O   | ALA | A | 377 | 9.077  | 39.325 | 75.312 | 1.00 | 27.36 |
| ATOM | 2962 | CB  | ALA | A | 377 | 6.091  | 38.433 | 74.891 | 1.00 | 26.74 |
| ATOM | 2963 | N   | TYR | A | 378 | 8.376  | 40.692 | 73.768 | 1.00 | 25.81 |
| ATOM | 2964 | CA  | TYR | A | 378 | 9.683  | 40.876 | 73.161 | 1.00 | 25.43 |
| ATOM | 2965 | C   | TYR | A | 378 | 10.862 | 41.194 | 74.057 | 1.00 | 30.49 |
| ATOM | 2966 | O   | TYR | A | 378 | 10.873 | 42.204 | 74.747 | 1.00 | 32.35 |
| ATOM | 2967 | CB  | TYR | A | 378 | 9.549  | 41.924 | 72.068 | 1.00 | 26.20 |
| ATOM | 2968 | CG  | TYR | A | 378 | 10.804 | 42.168 | 71.327 | 1.00 | 19.90 |
| ATOM | 2969 | CD1 | TYR | A | 378 | 11.256 | 41.231 | 70.406 | 1.00 | 18.53 |
| ATOM | 2970 | CD2 | TYR | A | 378 | 11.536 | 43.331 | 71.543 | 1.00 | 18.47 |
| ATOM | 2971 | CE1 | TYR | A | 378 | 12.444 | 41.436 | 69.716 | 1.00 | 15.98 |
| ATOM | 2972 | CE2 | TYR | A | 378 | 12.719 | 43.555 | 70.840 | 1.00 | 18.77 |
| ATOM | 2973 | CZ  | TYR | A | 378 | 13.161 | 42.609 | 69.920 | 1.00 | 16.37 |
| ATOM | 2974 | OH  | TYR | A | 378 | 14.309 | 42.811 | 69.212 | 1.00 | 32.30 |
| ATOM | 2975 | N   | SER | A | 379 | 11.879 | 40.317 | 73.977 | 1.00 | 23.03 |
| ATOM | 2976 | CA  | SER | A | 379 | 13.115 | 40.430 | 74.725 | 1.00 | 18.13 |
| ATOM | 2977 | C   | SER | A | 379 | 14.267 | 39.777 | 73.970 | 1.00 | 20.60 |
| ATOM | 2978 | O   | SER | A | 379 | 14.100 | 39.334 | 72.843 | 1.00 | 18.46 |
| ATOM | 2979 | CB  | SER | A | 379 | 12.976 | 39.740 | 76.067 | 1.00 | 23    |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 2998 | CB  | PRO | A | 382 | 13.777 | 34.514 | 71.351 | 1.00 | 17.20 |
| ATOM | 2999 | CG  | PRO | A | 382 | 13.003 | 35.618 | 72.033 | 1.00 | 18.32 |
| ATOM | 3000 | CD  | PRO | A | 382 | 13.627 | 35.873 | 73.399 | 1.00 | 12.12 |
| ATOM | 3001 | N   | TYR | A | 383 | 16.809 | 35.447 | 71.542 | 1.00 | 19.33 |
| ATOM | 3002 | CA  | TYR | A | 383 | 18.112 | 35.648 | 70.902 | 1.00 | 19.70 |
| ATOM | 3003 | C   | TYR | A | 383 | 19.246 | 34.953 | 71.651 | 1.00 | 28.79 |
| ATOM | 3004 | O   | TYR | A | 383 | 19.980 | 34.117 | 71.104 | 1.00 | 31.38 |
| ATOM | 3005 | CB  | TYR | A | 383 | 18.468 | 37.135 | 70.894 | 1.00 | 21.02 |
| ATOM | 3006 | CG  | TYR | A | 383 | 17.593 | 37.968 | 70.011 | 1.00 | 23.86 |
| ATOM | 3007 | CD1 | TYR | A | 383 | 16.290 | 38.277 | 70.404 | 1.00 | 28.36 |
| ATOM | 3008 | CD2 | TYR | A | 383 | 18.067 | 38.450 | 68.784 | 1.00 | 20.91 |
| ATOM | 3009 | CE1 | TYR | A | 383 | 15.473 | 39.054 | 69.576 | 1.00 | 30.88 |
| ATOM | 3010 | CE2 | TYR | A | 383 | 17.272 | 39.244 | 67.957 | 1.00 | 18.71 |
| ATOM | 3011 | CZ  | TYR | A | 383 | 15.967 | 39.533 | 68.358 | 1.00 | 25.95 |
| ATOM | 3012 | OH  | TYR | A | 383 | 15.171 | 40.294 | 67.556 | 1.00 | 30.84 |
| ATOM | 3013 | N   | GLU | A | 384 | 19.389 | 35.333 | 72.921 | 1.00 | 20.17 |
| ATOM | 3014 | CA  | GLU | A | 384 | 20.419 | 34.857 | 73.803 | 1.00 | 17.57 |
| ATOM | 3015 | C   | GLU | A | 384 | 20.188 | 33.506 | 74.405 | 1.00 | 22.88 |
| ATOM | 3016 | O   | GLU | A | 384 | 21.151 | 32.775 | 74.669 | 1.00 | 25.65 |
| ATOM | 3017 | CB  | GLU | A | 384 | 20.833 | 35.973 | 74.773 | 1.00 | 20.44 |
| ATOM | 3018 | CG  | GLU | A | 384 | 21.263 | 37.202 | 73.944 | 1.00 | 15.21 |
| ATOM | 3019 | CD  | GLU | A | 384 | 22.539 | 36.937 | 73.184 | 1.00 | 26.58 |
| ATOM | 3020 | OE1 | GLU | A | 384 | 23.185 | 35.915 | 73.293 | 1.00 | 17.84 |
| ATOM | 3021 | OE2 | GLU | A | 384 | 22.887 | 37.915 | 72.400 | 1.00 | 21.88 |
| ATOM | 3022 | N   | LYS | A | 385 | 18.935 | 33.116 | 74.610 | 1.00 | 20.33 |
| ATOM | 3023 | CA  | LYS | A | 385 | 18.736 | 31.767 | 75.146 | 1.00 | 20.05 |
| ATOM | 3024 | C   | LYS | A | 385 | 18.865 | 30.716 | 74.028 | 1.00 | 27.19 |
| ATOM | 3025 | O   | LYS | A | 385 | 19.420 | 29.621 | 74.219 | 1.00 | 31.66 |
| ATOM | 3026 | CB  | LYS | A | 385 | 17.507 | 31.577 | 76.014 | 1.00 | 21.51 |
| ATOM | 3027 | CG  | LYS | A | 385 | 17.676 | 30.384 | 76.953 | 1.00 | 22.29 |
| ATOM | 3028 | CD  | LYS | A | 385 | 16.386 | 29.820 | 77.518 | 1.00 | 19.87 |
| ATOM | 3029 | CE  | LYS | A | 385 | 16.049 | 30.277 | 78.937 | 1.00 | 31.60 |
| ATOM | 3030 | NZ  | LYS | A | 385 | 14.783 | 29.694 | 79.441 | 1.00 | 30.38 |
| ATOM | 3031 | N   | GLY | A | 386 | 18.364 | 31.084 | 72.832 | 1.00 | 20.72 |
| ATOM | 3032 | CA  | GLY | A | 386 | 18.453 | 30.248 | 71.637 | 1.00 | 17.41 |
| ATOM | 3033 | C   | GLY | A | 386 | 19.924 | 30.106 | 71.298 | 1.00 | 20.81 |
| ATOM | 3034 | O   | GLY | A | 386 | 20.396 | 29.001 | 71.225 | 1.00 | 22.50 |
| ATOM | 3035 | N   | PHE | A | 387 | 20.683 | 31.228 | 71.163 | 1.00 | 20.30 |
| ATOM | 3036 | CA  | PHE | A | 387 | 22.137 | 31.158 | 70.900 | 1.00 | 19.92 |
| ATOM | 3037 | C   | PHE | A | 387 | 22.840 | 30.263 | 71.905 | 1.00 | 29.09 |
| ATOM | 3038 | O   | PHE | A | 387 | 23.685 | 29.478 | 71.530 | 1.00 | 32.80 |
| ATOM | 3039 | CB  | PHE | A | 387 | 22.852 | 32.519 | 70.955 | 1.00 | 20.07 |
| ATOM | 3040 | CG  | PHE | A | 3   |        |        |        |      |       |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 3059 | N   | LEU | A | 390 | 22.217 | 26.659 | 71.262 | 1.00 | 24.49 |
| ATOM | 3060 | CA  | LEU | A | 390 | 23.050 | 26.340 | 70.107 | 1.00 | 25.05 |
| ATOM | 3061 | C   | LEU | A | 390 | 24.531 | 26.256 | 70.383 | 1.00 | 32.31 |
| ATOM | 3062 | O   | LEU | A | 390 | 25.183 | 25.301 | 69.932 | 1.00 | 33.60 |
| ATOM | 3063 | CB  | LEU | A | 390 | 22.765 | 27.152 | 68.844 | 1.00 | 23.33 |
| ATOM | 3064 | CG  | LEU | A | 390 | 21.307 | 27.026 | 68.442 | 1.00 | 23.38 |
| ATOM | 3065 | CD1 | LEU | A | 390 | 20.986 | 28.025 | 67.334 | 1.00 | 20.84 |
| ATOM | 3066 | CD2 | LEU | A | 390 | 20.988 | 25.591 | 68.017 | 1.00 | 18.86 |
| ATOM | 3067 | N   | PHE | A | 391 | 25.058 | 27.231 | 71.127 | 1.00 | 28.52 |
| ATOM | 3068 | CA  | PHE | A | 391 | 26.480 | 27.236 | 71.494 | 1.00 | 27.82 |
| ATOM | 3069 | C   | PHE | A | 391 | 26.813 | 25.992 | 72.312 | 1.00 | 28.67 |
| ATOM | 3070 | O   | PHE | A | 391 | 27.839 | 25.331 | 72.148 | 1.00 | 26.96 |
| ATOM | 3071 | CB  | PHE | A | 391 | 26.834 | 28.455 | 72.341 | 1.00 | 28.60 |
| ATOM | 3072 | CG  | PHE | A | 391 | 28.296 | 28.786 | 72.283 | 1.00 | 30.53 |
| ATOM | 3073 | CD1 | PHE | A | 391 | 28.967 | 28.816 | 71.064 | 1.00 | 35.08 |
| ATOM | 3074 | CD2 | PHE | A | 391 | 29.020 | 29.063 | 73.440 | 1.00 | 36.52 |
| ATOM | 3075 | CE1 | PHE | A | 391 | 30.320 | 29.142 | 70.983 | 1.00 | 37.61 |
| ATOM | 3076 | CE2 | PHE | A | 391 | 30.378 | 29.383 | 73.382 | 1.00 | 40.61 |
| ATOM | 3077 | CZ  | PHE | A | 391 | 31.026 | 29.432 | 72.148 | 1.00 | 37.64 |
| ATOM | 3078 | N   | TYR | A | 392 | 25.913 | 25.699 | 73.225 | 1.00 | 24.90 |
| ATOM | 3079 | CA  | TYR | A | 392 | 26.044 | 24.550 | 74.065 | 1.00 | 24.66 |
| ATOM | 3080 | C   | TYR | A | 392 | 26.106 | 23.298 | 73.186 | 1.00 | 34.30 |
| ATOM | 3081 | O   | TYR | A | 392 | 27.058 | 22.558 | 73.268 | 1.00 | 37.51 |
| ATOM | 3082 | CB  | TYR | A | 392 | 24.821 | 24.501 | 74.967 | 1.00 | 26.39 |
| ATOM | 3083 | CG  | TYR | A | 392 | 24.631 | 23.181 | 75.678 | 1.00 | 31.99 |
| ATOM | 3084 | CD1 | TYR | A | 392 | 25.546 | 22.715 | 76.625 | 1.00 | 35.17 |
| ATOM | 3085 | CD2 | TYR | A | 392 | 23.501 | 22.397 | 75.432 | 1.00 | 32.49 |
| ATOM | 3086 | CE1 | TYR | A | 392 | 25.341 | 21.512 | 77.306 | 1.00 | 39.01 |
| ATOM | 3087 | CE2 | TYR | A | 392 | 23.281 | 21.184 | 76.094 | 1.00 | 31.50 |
| ATOM | 3088 | CZ  | TYR | A | 392 | 24.206 | 20.743 | 77.035 | 1.00 | 34.08 |
| ATOM | 3089 | OH  | TYR | A | 392 | 23.986 | 19.564 | 77.683 | 1.00 | 36.46 |
| ATOM | 3090 | N   | LEU | A | 393 | 25.101 | 23.067 | 72.310 | 1.00 | 31.02 |
| ATOM | 3091 | CA  | LEU | A | 393 | 25.043 | 21.889 | 71.410 | 1.00 | 29.65 |
| ATOM | 3092 | C   | LEU | A | 393 | 26.274 | 21.616 | 70.507 | 1.00 | 32.03 |
| ATOM | 3093 | O   | LEU | A | 393 | 26.664 | 20.468 | 70.267 | 1.00 | 27.90 |
| ATOM | 3094 | CB  | LEU | A | 393 | 23.758 | 21.905 | 70.552 | 1.00 | 28.85 |
| ATOM | 3095 | CG  | LEU | A | 393 | 22.489 | 21.688 | 71.375 | 1.00 | 30.33 |
| ATOM | 3096 | CD1 | LEU | A | 393 | 21.256 | 22.047 | 70.559 | 1.00 | 27.38 |
| ATOM | 3097 | CD2 | LEU | A | 393 | 22.400 | 20.246 | 71.865 | 1.00 | 29.76 |
| ATOM | 3098 | N   | GLU | A | 394 | 26.841 | 22.701 | 69.980 | 1.00 | 30.84 |
| ATOM | 3099 | CA  | GLU | A | 394 | 28.000 | 22.727 | 69.118 | 1.00 | 30.05 |
| ATOM | 3100 | C   | GLU | A | 394 | 29.210 | 22.214 | 69.868 | 1.00 | 39.16 |
| ATOM | 3101 | O   | GLU | A |     |        |        |        |      |       |



601210-0269

|      |      |     |           |        |        |        |      |        |
|------|------|-----|-----------|--------|--------|--------|------|--------|
| ATOM | 3120 | CB  | LEU A 396 | 27.055 | 19.072 | 73.628 | 1.00 | 37.93  |
| ATOM | 3121 | CG  | LEU A 396 | 26.389 | 17.732 | 73.946 | 1.00 | 42.72  |
| ATOM | 3122 | CD1 | LEU A 396 | 26.436 | 17.489 | 75.445 | 1.00 | 45.42  |
| ATOM | 3123 | CD2 | LEU A 396 | 24.917 | 17.709 | 73.527 | 1.00 | 43.81  |
| ATOM | 3124 | N   | LEU A 397 | 28.303 | 18.456 | 70.730 | 1.00 | 28.48  |
| ATOM | 3125 | CA  | LEU A 397 | 28.337 | 17.595 | 69.589 | 1.00 | 25.49  |
| ATOM | 3126 | C   | LEU A 397 | 29.620 | 17.609 | 68.771 | 1.00 | 36.86  |
| ATOM | 3127 | O   | LEU A 397 | 29.596 | 17.220 | 67.599 | 1.00 | 39.85  |
| ATOM | 3128 | CB  | LEU A 397 | 27.156 | 17.924 | 68.686 | 1.00 | 23.73  |
| ATOM | 3129 | CG  | LEU A 397 | 25.843 | 17.773 | 69.401 | 1.00 | 25.82  |
| ATOM | 3130 | CD1 | LEU A 397 | 24.740 | 18.559 | 68.669 | 1.00 | 22.99  |
| ATOM | 3131 | CD2 | LEU A 397 | 25.525 | 16.272 | 69.452 | 1.00 | 27.30  |
| ATOM | 3132 | N   | GLY A 398 | 30.731 | 18.069 | 69.342 | 1.00 | 33.98  |
| ATOM | 3133 | CA  | GLY A 398 | 31.993 | 18.038 | 68.617 | 1.00 | 34.14  |
| ATOM | 3134 | C   | GLY A 398 | 32.547 | 19.260 | 67.889 | 1.00 | 38.92  |
| ATOM | 3135 | O   | GLY A 398 | 33.502 | 19.097 | 67.115 | 1.00 | 39.98  |
| ATOM | 3136 | N   | GLY A 399 | 32.001 | 20.457 | 68.105 | 1.00 | 33.01  |
| ATOM | 3137 | CA  | GLY A 399 | 32.543 | 21.650 | 67.440 | 1.00 | 30.35  |
| ATOM | 3138 | C   | GLY A 399 | 31.713 | 22.336 | 66.365 | 1.00 | 31.72  |
| ATOM | 3139 | O   | GLY A 399 | 30.800 | 21.823 | 65.762 | 1.00 | 34.57  |
| ATOM | 3140 | N   | PRO A 400 | 32.076 | 23.550 | 66.124 | 1.00 | 33.01  |
| ATOM | 3141 | CA  | PRO A 400 | 31.429 | 24.406 | 65.151 | 1.00 | 35.02  |
| ATOM | 3142 | C   | PRO A 400 | 31.379 | 23.794 | 63.750 | 1.00 | 43.93  |
| ATOM | 3143 | O   | PRO A 400 | 30.360 | 23.838 | 63.045 | 1.00 | 40.14  |
| ATOM | 3144 | CB  | PRO A 400 | 32.293 | 25.672 | 65.111 | 1.00 | 35.73  |
| ATOM | 3145 | CG  | PRO A 400 | 33.539 | 25.411 | 65.948 | 1.00 | 38.03  |
| ATOM | 3146 | CD  | PRO A 400 | 33.423 | 24.010 | 66.517 | 1.00 | 33.92  |
| ATOM | 3147 | N   | GLU A 401 | 32.512 | 23.237 | 63.345 | 1.00 | 43.85  |
| ATOM | 3148 | CA  | GLU A 401 | 32.597 | 22.620 | 62.042 | 1.00 | 42.92  |
| ATOM | 3149 | C   | GLU A 401 | 31.491 | 21.587 | 61.878 | 1.00 | 37.92  |
| ATOM | 3150 | O   | GLU A 401 | 30.810 | 21.588 | 60.866 | 1.00 | 33.79  |
| ATOM | 3151 | CB  | GLU A 401 | 33.996 | 22.034 | 61.789 | 1.00 | 45.93  |
| ATOM | 3152 | CG  | GLU A 401 | 34.578 | 22.372 | 60.398 | 1.00 | 69.62  |
| ATOM | 3153 | CD  | GLU A 401 | 35.603 | 21.373 | 59.911 | 1.00 | 100.00 |
| ATOM | 3154 | OE1 | GLU A 401 | 36.702 | 21.236 | 60.427 | 1.00 | 100.00 |
| ATOM | 3155 | OE2 | GLU A 401 | 35.195 | 20.689 | 58.865 | 1.00 | 93.16  |
| ATOM | 3156 | N   | ILE A 402 | 31.317 | 20.720 | 62.902 | 1.00 | 34.58  |
| ATOM | 3157 | CA  | ILE A 402 | 30.281 | 19.681 | 62.922 | 1.00 | 33.20  |
| ATOM | 3158 | C   | ILE A 402 | 28.898 | 20.291 | 62.938 | 1.00 | 39.09  |
| ATOM | 3159 | O   | ILE A 402 | 28.065 | 19.896 | 62.133 | 1.00 | 41.43  |
| ATOM | 3160 | CB  | ILE A 402 | 30.391 | 18.673 | 64.078 | 1.00 | 33.82  |
| ATOM | 3161 | CG1 | ILE A 402 | 31.490 | 17.661 | 63.811 | 1.00 | 34.70  |
| ATOM | 3162 | CG2 | ILE A 402 | 29.080 | 17.900 | 64.287 | 1.00 | 23.32  |
| ATOM | 3163 | CD1 | ILE A 402 | 31.878 | 16.896 | 65.080 | 1.00 | 49.20  |
| ATOM | 3164 | N   | PHE A 403 | 28.668 | 21.246 | 63.868 | 1.00 | 32.73  |
| ATOM | 3165 | CA  | PHE A 403 | 27.390 | 21.952 | 64.044 | 1.00 | 29.52  |
| ATOM | 3166 | C   | PHE A 403 | 27.032 | 22.816 | 62.836 | 1.00 | 33.94  |
| ATOM | 3167 | O   | PHE A 403 | 25.866 | 23.022 | 62.469 | 1.00 | 34.15  |
| ATOM | 3168 | CB  | PHE A 403 | 27.319 | 22.719 | 65.381 | 1.00 | 29.03  |
| ATOM | 3169 | CG  | PHE A 403 | 25.917 | 22.783 | 65.929 | 1.00 | 28.54  |
| ATOM | 3170 | CD1 | PHE A 403 | 25.323 | 21.643 | 66.484 | 1.00 | 29.91  |
| ATOM | 3171 | CD2 | PHE A 403 | 25.176 | 23.964 | 65.873 | 1.00 | 27.62  |
| ATOM | 3172 | CE1 | PHE A 403 | 24.021 | 21.667 | 66.990 | 1.00 | 27.38  |
| ATOM | 3173 | CE2 | PHE A 403 | 23.881 | 24.017 | 66.393 | 1.00 | 28.82  |
| ATOM | 3174 | CZ  | PHE A 403 | 23.304 | 22.863 | 66.932 | 1.00 | 25.72  |
| ATOM | 3175 | N   | LEU A 404 | 28.040 | 23.327 | 62.165 | 1.00 | 31.31  |
| ATOM | 3176 | CA  | LEU A 404 | 27.687 | 24.080 | 60.983 | 1.00 | 32.95  |
| ATOM | 3177 | C   | LEU A 404 | 27.068 | 23.099 | 59.952 | 1.00 | 32.89  |
| ATOM | 3178 | O   | LEU A 404 | 26.050 | 23.361 | 59.315 | 1.00 | 37.36  |
| ATOM | 3179 | CB  | LEU A 404 | 28.798 | 25.045 | 60.464 | 1.00 | 33.15  |
| ATOM | 3180 | CG  | LEU A 404 | 29.029 | 26.208 | 61.444 | 1.00 | 36.96  |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 3181 | CD1 | LEU | A | 404 | 30.454 | 26.717 | 61.353 | 1.00 | 37.13 |
| ATOM | 3182 | CD2 | LEU | A | 404 | 28.083 | 27.362 | 61.163 | 1.00 | 39.27 |
| ATOM | 3183 | N   | GLY | A | 405 | 27.670 | 21.921 | 59.826 | 1.00 | 22.02 |
| ATOM | 3184 | CA  | GLY | A | 405 | 27.167 | 20.908 | 58.928 | 1.00 | 22.77 |
| ATOM | 3185 | C   | GLY | A | 405 | 25.698 | 20.676 | 59.206 | 1.00 | 31.85 |
| ATOM | 3186 | O   | GLY | A | 405 | 24.885 | 20.438 | 58.297 | 1.00 | 33.01 |
| ATOM | 3187 | N   | PHE | A | 406 | 25.364 | 20.747 | 60.493 | 1.00 | 26.28 |
| ATOM | 3188 | CA  | PHE | A | 406 | 23.992 | 20.565 | 60.863 | 1.00 | 25.27 |
| ATOM | 3189 | C   | PHE | A | 406 | 23.188 | 21.757 | 60.365 | 1.00 | 34.80 |
| ATOM | 3190 | O   | PHE | A | 406 | 22.195 | 21.629 | 59.638 | 1.00 | 36.22 |
| ATOM | 3191 | CB  | PHE | A | 406 | 23.798 | 20.268 | 62.351 | 1.00 | 24.52 |
| ATOM | 3192 | CG  | PHE | A | 406 | 22.388 | 20.525 | 62.798 | 1.00 | 24.82 |
| ATOM | 3193 | CD1 | PHE | A | 406 | 21.328 | 19.734 | 62.353 | 1.00 | 28.50 |
| ATOM | 3194 | CD2 | PHE | A | 406 | 22.107 | 21.579 | 63.669 | 1.00 | 30.12 |
| ATOM | 3195 | CE1 | PHE | A | 406 | 20.025 | 19.977 | 62.793 | 1.00 | 31.40 |
| ATOM | 3196 | CE2 | PHE | A | 406 | 20.810 | 21.862 | 64.105 | 1.00 | 32.57 |
| ATOM | 3197 | CZ  | PHE | A | 406 | 19.771 | 21.037 | 63.669 | 1.00 | 31.88 |
| ATOM | 3198 | N   | LEU | A | 407 | 23.661 | 22.934 | 60.708 | 1.00 | 32.11 |
| ATOM | 3199 | CA  | LEU | A | 407 | 22.972 | 24.132 | 60.269 | 1.00 | 33.11 |
| ATOM | 3200 | C   | LEU | A | 407 | 22.706 | 24.204 | 58.767 | 1.00 | 34.74 |
| ATOM | 3201 | O   | LEU | A | 407 | 21.635 | 24.615 | 58.341 | 1.00 | 35.21 |
| ATOM | 3202 | CB  | LEU | A | 407 | 23.589 | 25.420 | 60.840 | 1.00 | 35.36 |
| ATOM | 3203 | CG  | LEU | A | 407 | 22.597 | 26.577 | 60.855 | 1.00 | 41.79 |
| ATOM | 3204 | CD1 | LEU | A | 407 | 23.048 | 27.626 | 61.833 | 1.00 | 40.45 |
| ATOM | 3205 | CD2 | LEU | A | 407 | 22.513 | 27.197 | 59.461 | 1.00 | 49.57 |
| ATOM | 3206 | N   | LYS | A | 408 | 23.667 | 23.804 | 57.948 | 1.00 | 34.92 |
| ATOM | 3207 | CA  | LYS | A | 408 | 23.476 | 23.826 | 56.490 | 1.00 | 36.29 |
| ATOM | 3208 | C   | LYS | A | 408 | 22.378 | 22.876 | 56.037 | 1.00 | 38.15 |
| ATOM | 3209 | O   | LYS | A | 408 | 21.568 | 23.191 | 55.160 | 1.00 | 35.09 |
| ATOM | 3210 | CB  | LYS | A | 408 | 24.747 | 23.517 | 55.707 | 1.00 | 40.54 |
| ATOM | 3211 | CG  | LYS | A | 408 | 24.633 | 23.873 | 54.214 | 1.00 | 43.41 |
| ATOM | 3212 | CD  | LYS | A | 408 | 25.950 | 23.796 | 53.422 | 1.00 | 49.26 |
| ATOM | 3213 | CE  | LYS | A | 408 | 26.808 | 25.059 | 53.459 | 1.00 | 61.45 |
| ATOM | 3214 | NZ  | LYS | A | 408 | 28.014 | 24.994 | 52.606 | 1.00 | 73.78 |
| ATOM | 3215 | N   | ALA | A | 409 | 22.352 | 21.690 | 56.655 | 1.00 | 35.34 |
| ATOM | 3216 | CA  | ALA | A | 409 | 21.333 | 20.698 | 56.298 | 1.00 | 36.14 |
| ATOM | 3217 | C   | ALA | A | 409 | 19.927 | 21.041 | 56.814 | 1.00 | 38.45 |
| ATOM | 3218 | O   | ALA | A | 409 | 18.913 | 20.821 | 56.134 | 1.00 | 37.39 |
| ATOM | 3219 | CB  | ALA | A | 409 | 21.762 | 19.273 | 56.626 | 1.00 | 36.66 |
| ATOM | 3220 | N   | TYR | A | 410 | 19.902 | 21.597 | 58.030 | 1.00 | 33.14 |
| ATOM | 3221 | CA  | TYR | A | 410 | 18.693 | 22.059 | 58.682 | 1.00 | 29.65 |
| ATOM | 3222 | C   | TYR | A | 410 | 18.028 | 23.051 | 57.730 | 1.00 | 35.55 |
| ATOM | 3223 | O   | TYR | A | 410 | 1      |        |        |      |       |



50122410 022599

|      |      |     |     |   |     |        |        |        |      |        |
|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
| ATOM | 3242 | O   | GLU | A | 412 | 16.182 | 22.225 | 52.531 | 1.00 | 31.89  |
| ATOM | 3243 | CB  | GLU | A | 412 | 19.502 | 21.883 | 52.932 | 1.00 | 36.48  |
| ATOM | 3244 | CG  | GLU | A | 412 | 20.443 | 22.174 | 51.737 | 1.00 | 67.01  |
| ATOM | 3245 | CD  | GLU | A | 412 | 21.872 | 21.699 | 51.962 | 1.00 | 100.00 |
| ATOM | 3246 | OE1 | GLU | A | 412 | 22.193 | 20.782 | 52.716 | 1.00 | 100.00 |
| ATOM | 3247 | OE2 | GLU | A | 412 | 22.750 | 22.396 | 51.277 | 1.00 | 94.73  |
| ATOM | 3248 | N   | LYS | A | 413 | 16.922 | 21.444 | 54.444 | 1.00 | 22.18  |
| ATOM | 3249 | CA  | LYS | A | 413 | 15.729 | 20.692 | 54.714 | 1.00 | 17.91  |
| ATOM | 3250 | C   | LYS | A | 413 | 14.463 | 21.486 | 54.855 | 1.00 | 23.75  |
| ATOM | 3251 | O   | LYS | A | 413 | 13.417 | 20.978 | 54.503 | 1.00 | 25.92  |
| ATOM | 3252 | CB  | LYS | A | 413 | 15.890 | 19.911 | 55.988 | 1.00 | 15.65  |
| ATOM | 3253 | CG  | LYS | A | 413 | 14.554 | 19.422 | 56.503 | 1.00 | 38.69  |
| ATOM | 3254 | CD  | LYS | A | 413 | 14.150 | 18.089 | 55.903 | 1.00 | 58.11  |
| ATOM | 3255 | CE  | LYS | A | 413 | 13.634 | 17.099 | 56.937 | 1.00 | 64.98  |
| ATOM | 3256 | NZ  | LYS | A | 413 | 13.457 | 15.751 | 56.381 | 1.00 | 73.89  |
| ATOM | 3257 | N   | PHE | A | 414 | 14.530 | 22.688 | 55.424 | 1.00 | 25.40  |
| ATOM | 3258 | CA  | PHE | A | 414 | 13.316 | 23.479 | 55.640 | 1.00 | 27.80  |
| ATOM | 3259 | C   | PHE | A | 414 | 13.151 | 24.748 | 54.821 | 1.00 | 35.82  |
| ATOM | 3260 | O   | PHE | A | 414 | 12.276 | 25.557 | 55.122 | 1.00 | 35.17  |
| ATOM | 3261 | CB  | PHE | A | 414 | 13.063 | 23.791 | 57.118 | 1.00 | 30.46  |
| ATOM | 3262 | CG  | PHE | A | 414 | 12.936 | 22.553 | 57.964 | 1.00 | 33.88  |
| ATOM | 3263 | CD1 | PHE | A | 414 | 11.746 | 21.826 | 57.996 | 1.00 | 35.94  |
| ATOM | 3264 | CD2 | PHE | A | 414 | 14.005 | 22.110 | 58.742 | 1.00 | 37.75  |
| ATOM | 3265 | CE1 | PHE | A | 414 | 11.629 | 20.664 | 58.761 | 1.00 | 37.77  |
| ATOM | 3266 | CE2 | PHE | A | 414 | 13.888 | 20.962 | 59.526 | 1.00 | 42.23  |
| ATOM | 3267 | CZ  | PHE | A | 414 | 12.698 | 20.231 | 59.542 | 1.00 | 39.10  |
| ATOM | 3268 | N   | SER | A | 415 | 13.970 | 24.933 | 53.795 | 1.00 | 36.12  |
| ATOM | 3269 | CA  | SER | A | 415 | 13.858 | 26.115 | 52.945 | 1.00 | 36.36  |
| ATOM | 3270 | C   | SER | A | 415 | 12.412 | 26.295 | 52.510 | 1.00 | 38.99  |
| ATOM | 3271 | O   | SER | A | 415 | 11.730 | 25.315 | 52.243 | 1.00 | 41.04  |
| ATOM | 3272 | CB  | SER | A | 415 | 14.773 | 26.008 | 51.736 | 1.00 | 37.43  |
| ATOM | 3273 | OG  | SER | A | 415 | 16.036 | 26.566 | 52.046 | 1.00 | 46.73  |
| ATOM | 3274 | N   | TYR | A | 416 | 11.928 | 27.537 | 52.475 | 1.00 | 33.40  |
| ATOM | 3275 | CA  | TYR | A | 416 | 10.541 | 27.832 | 52.072 | 1.00 | 30.88  |
| ATOM | 3276 | C   | TYR | A | 416 | 9.453  | 27.183 | 52.947 | 1.00 | 33.62  |
| ATOM | 3277 | O   | TYR | A | 416 | 8.295  | 27.095 | 52.546 | 1.00 | 33.44  |
| ATOM | 3278 | CB  | TYR | A | 416 | 10.292 | 27.479 | 50.584 | 1.00 | 28.42  |
| ATOM | 3279 | CG  | TYR | A | 416 | 11.496 | 27.782 | 49.723 | 1.00 | 24.76  |
| ATOM | 3280 | CD1 | TYR | A | 416 | 11.791 | 29.087 | 49.338 | 1.00 | 26.55  |
| ATOM | 3281 | CD2 | TYR | A | 416 | 12.375 | 26.778 | 49.335 | 1.00 | 21.68  |
| ATOM | 3282 | CE1 | TYR | A | 416 | 12.914 | 29.384 | 48.570 | 1.00 | 25.16  |
| ATOM | 3283 | CE2 | TYR | A | 416 | 13.504 | 27.052 | 48.572 | 1.00 | 20.15  |
| ATOM | 3284 | CZ  | TYR | A | 416 | 13.780 | 28.360 | 48.189 | 1.00 | 30.62  |
| ATOM | 3285 | OH  | TYR | A | 416 | 14.892 | 28.616 | 47.399 | 1.00 | 35.15  |
| ATOM | 3286 | N   | LYS | A | 417 | 9.823  | 26.713 | 54.122 | 1.00 | 27.67  |
| ATOM | 3287 | CA  | LYS | A | 417 | 8.889  | 26.065 | 55.008 | 1.00 | 28.02  |
| ATOM | 3288 | C   | LYS | A | 417 | 8.733  | 26.830 | 56.317 | 1.00 | 31.36  |
| ATOM | 3289 | O   | LYS | A | 417 | 9.547  | 27.671 | 56.682 | 1.00 | 33.15  |
| ATOM | 3290 | CB  | LYS | A | 417 | 9.335  | 24.615 | 55.252 | 1.00 | 33.86  |
| ATOM | 3291 | CG  | LYS | A | 417 | 8.449  | 23.792 | 56.201 | 1.00 | 86.28  |
| ATOM | 3292 | CD  | LYS | A | 417 | 8.742  | 22.275 | 56.232 | 1.00 | 100.00 |
| ATOM | 3293 | CE  | LYS | A | 417 | 7.924  | 21.471 | 57.265 | 1.00 | 72.28  |
| ATOM | 3294 | NZ  | LYS | A | 417 | 8.280  | 20.033 | 57.323 | 1.00 | 41.88  |
| ATOM | 3295 | N   | SER | A | 418 | 7.668  | 26.557 | 57.033 | 1.00 | 28.88  |
| ATOM | 3296 | CA  | SER | A | 418 | 7.455  | 27.195 | 58.335 | 1.00 | 30.04  |
| ATOM | 3297 | C   | SER | A | 418 | 7.425  | 26.064 | 59.332 | 1.00 | 34.09  |
| ATOM | 3298 | O   | SER | A | 418 | 6.614  | 25.145 | 59.193 | 1.00 | 31.54  |
| ATOM | 3299 | CB  | SER | A | 418 | 6.261  | 28.126 | 58.410 | 1.00 | 31.46  |
| ATOM | 3300 | OG  | SER | A | 418 | 6.417  | 29.106 | 57.399 | 1.00 | 35.01  |
| ATOM | 3301 | N   | ILE | A | 419 | 8.356  | 26.077 | 60.281 | 1.00 | 28.50  |
| ATOM | 3302 | CA  | ILE | A | 419 | 8.446  | 24.971 | 61.205 | 1.00 | 23.86  |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 3303 | C   | ILE | A | 419 | 8.272  | 25.342 | 62.641 | 1.00 | 25.06 |
| ATOM | 3304 | O   | ILE | A | 419 | 8.122  | 26.500 | 63.002 | 1.00 | 21.64 |
| ATOM | 3305 | CB  | ILE | A | 419 | 9.803  | 24.314 | 61.026 | 1.00 | 25.02 |
| ATOM | 3306 | CG1 | ILE | A | 419 | 10.863 | 25.325 | 61.399 | 1.00 | 23.63 |
| ATOM | 3307 | CG2 | ILE | A | 419 | 10.051 | 23.937 | 59.565 | 1.00 | 23.22 |
| ATOM | 3308 | CD1 | ILE | A | 419 | 12.236 | 24.688 | 61.253 | 1.00 | 23.48 |
| ATOM | 3309 | N   | THR | A | 420 | 8.321  | 24.302 | 63.455 | 1.00 | 24.71 |
| ATOM | 3310 | CA  | THR | A | 420 | 8.201  | 24.417 | 64.895 | 1.00 | 24.36 |
| ATOM | 3311 | C   | THR | A | 420 | 9.416  | 23.795 | 65.538 | 1.00 | 28.90 |
| ATOM | 3312 | O   | THR | A | 420 | 10.190 | 23.112 | 64.863 | 1.00 | 23.38 |
| ATOM | 3313 | CB  | THR | A | 420 | 6.979  | 23.691 | 65.448 | 1.00 | 24.92 |
| ATOM | 3314 | OG1 | THR | A | 420 | 7.190  | 22.313 | 65.291 | 1.00 | 26.43 |
| ATOM | 3315 | CG2 | THR | A | 420 | 5.728  | 24.082 | 64.694 | 1.00 | 31.57 |
| ATOM | 3316 | N   | THR | A | 421 | 9.542  | 24.051 | 66.855 | 1.00 | 29.30 |
| ATOM | 3317 | CA  | THR | A | 421 | 10.610 | 23.549 | 67.709 | 1.00 | 27.78 |
| ATOM | 3318 | C   | THR | A | 421 | 10.831 | 22.035 | 67.585 | 1.00 | 30.99 |
| ATOM | 3319 | O   | THR | A | 421 | 11.975 | 21.594 | 67.489 | 1.00 | 33.28 |
| ATOM | 3320 | CB  | THR | A | 421 | 10.394 | 23.969 | 69.166 | 1.00 | 21.94 |
| ATOM | 3321 | OG1 | THR | A | 421 | 10.567 | 25.369 | 69.263 | 1.00 | 24.52 |
| ATOM | 3322 | CG2 | THR | A | 421 | 11.399 | 23.221 | 70.045 | 1.00 | 20.12 |
| ATOM | 3323 | N   | ASP | A | 422 | 9.721  | 21.272 | 67.575 | 1.00 | 21.94 |
| ATOM | 3324 | CA  | ASP | A | 422 | 9.706  | 19.823 | 67.430 | 1.00 | 21.08 |
| ATOM | 3325 | C   | ASP | A | 422 | 10.323 | 19.401 | 66.104 | 1.00 | 31.16 |
| ATOM | 3326 | O   | ASP | A | 422 | 11.110 | 18.427 | 66.027 | 1.00 | 31.95 |
| ATOM | 3327 | CB  | ASP | A | 422 | 8.276  | 19.278 | 67.561 | 1.00 | 19.49 |
| ATOM | 3328 | CG  | ASP | A | 422 | 8.236  | 17.802 | 67.298 | 1.00 | 31.85 |
| ATOM | 3329 | OD1 | ASP | A | 422 | 9.130  | 17.040 | 67.654 | 1.00 | 29.73 |
| ATOM | 3330 | OD2 | ASP | A | 422 | 7.197  | 17.415 | 66.598 | 1.00 | 56.60 |
| ATOM | 3331 | N   | ASP | A | 423 | 9.957  | 20.146 | 65.049 | 1.00 | 26.75 |
| ATOM | 3332 | CA  | ASP | A | 423 | 10.505 | 19.876 | 63.729 | 1.00 | 26.01 |
| ATOM | 3333 | C   | ASP | A | 423 | 12.027 | 19.957 | 63.830 | 1.00 | 40.09 |
| ATOM | 3334 | O   | ASP | A | 423 | 12.753 | 19.020 | 63.500 | 1.00 | 47.09 |
| ATOM | 3335 | CB  | ASP | A | 423 | 10.000 | 20.833 | 62.631 | 1.00 | 24.86 |
| ATOM | 3336 | CG  | ASP | A | 423 | 8.538  | 20.722 | 62.343 | 1.00 | 39.90 |
| ATOM | 3337 | OD1 | ASP | A | 423 | 7.968  | 19.649 | 62.299 | 1.00 | 45.03 |
| ATOM | 3338 | OD2 | ASP | A | 423 | 7.943  | 21.887 | 62.113 | 1.00 | 40.43 |
| ATOM | 3339 | N   | TRP | A | 424 | 12.493 | 21.099 | 64.320 | 1.00 | 31.92 |
| ATOM | 3340 | CA  | TRP | A | 424 | 13.903 | 21.372 | 64.495 | 1.00 | 29.69 |
| ATOM | 3341 | C   | TRP | A | 424 | 14.611 | 20.271 | 65.282 | 1.00 | 33.81 |
| ATOM | 3342 | O   | TRP | A | 424 | 15.537 | 19.616 | 64.824 | 1.00 | 35.87 |
| ATOM | 3343 | CB  | TRP | A | 424 | 14.056 | 22.711 | 65.239 | 1.00 | 26.11 |
| ATOM | 3344 | CG  | TRP | A | 424 | 15.431 | 22.869 | 65.786 | 1.00 | 27.05 |
| ATOM | 3345 | CD1 | TRP | A | 424 | 16.518 | 23.302 | 65.101 | 1.0  |       |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 3364 | C   | ASP | A | 426 | 14.453 | 15.879 | 64.387 | 1.00 | 28.33 |
| ATOM | 3365 | O   | ASP | A | 426 | 15.070 | 14.832 | 64.232 | 1.00 | 31.25 |
| ATOM | 3366 | CB  | ASP | A | 426 | 11.920 | 15.840 | 65.098 | 1.00 | 19.79 |
| ATOM | 3367 | CG  | ASP | A | 426 | 10.998 | 15.575 | 66.274 | 1.00 | 25.54 |
| ATOM | 3368 | OD1 | ASP | A | 426 | 11.341 | 15.466 | 67.409 | 1.00 | 29.73 |
| ATOM | 3369 | OD2 | ASP | A | 426 | 9.804  | 15.611 | 65.938 | 1.00 | 20.67 |
| ATOM | 3370 | N   | PHE | A | 427 | 14.674 | 16.926 | 63.612 | 1.00 | 25.09 |
| ATOM | 3371 | CA  | PHE | A | 427 | 15.654 | 16.899 | 62.540 | 1.00 | 25.81 |
| ATOM | 3372 | C   | PHE | A | 427 | 17.066 | 16.718 | 63.159 | 1.00 | 34.01 |
| ATOM | 3373 | O   | PHE | A | 427 | 17.843 | 15.851 | 62.773 | 1.00 | 36.25 |
| ATOM | 3374 | CB  | PHE | A | 427 | 15.589 | 18.197 | 61.704 | 1.00 | 26.35 |
| ATOM | 3375 | CG  | PHE | A | 427 | 16.698 | 18.202 | 60.702 | 1.00 | 27.40 |
| ATOM | 3376 | CD1 | PHE | A | 427 | 16.714 | 17.247 | 59.686 | 1.00 | 29.97 |
| ATOM | 3377 | CD2 | PHE | A | 427 | 17.773 | 19.084 | 60.805 | 1.00 | 28.71 |
| ATOM | 3378 | CE1 | PHE | A | 427 | 17.730 | 17.194 | 58.733 | 1.00 | 27.72 |
| ATOM | 3379 | CE2 | PHE | A | 427 | 18.806 | 19.046 | 59.867 | 1.00 | 30.37 |
| ATOM | 3380 | CZ  | PHE | A | 427 | 18.780 | 18.104 | 58.837 | 1.00 | 26.34 |
| ATOM | 3381 | N   | LEU | A | 428 | 17.369 | 17.544 | 64.160 | 1.00 | 28.94 |
| ATOM | 3382 | CA  | LEU | A | 428 | 18.622 | 17.496 | 64.924 | 1.00 | 27.74 |
| ATOM | 3383 | C   | LEU | A | 428 | 18.989 | 16.047 | 65.303 | 1.00 | 32.08 |
| ATOM | 3384 | O   | LEU | A | 428 | 20.145 | 15.647 | 65.209 | 1.00 | 36.38 |
| ATOM | 3385 | CB  | LEU | A | 428 | 18.510 | 18.362 | 66.223 | 1.00 | 24.68 |
| ATOM | 3386 | CG  | LEU | A | 428 | 19.778 | 18.377 | 67.079 | 1.00 | 24.30 |
| ATOM | 3387 | CD1 | LEU | A | 428 | 20.855 | 19.278 | 66.467 | 1.00 | 23.00 |
| ATOM | 3388 | CD2 | LEU | A | 428 | 19.446 | 18.856 | 68.481 | 1.00 | 16.41 |
| ATOM | 3389 | N   | TYR | A | 429 | 17.991 | 15.271 | 65.735 | 1.00 | 23.71 |
| ATOM | 3390 | CA  | TYR | A | 429 | 18.148 | 13.896 | 66.144 | 1.00 | 23.18 |
| ATOM | 3391 | C   | TYR | A | 429 | 18.311 | 12.967 | 64.976 | 1.00 | 26.62 |
| ATOM | 3392 | O   | TYR | A | 429 | 18.911 | 11.910 | 65.076 | 1.00 | 28.43 |
| ATOM | 3393 | CB  | TYR | A | 429 | 16.921 | 13.453 | 66.914 | 1.00 | 25.59 |
| ATOM | 3394 | CG  | TYR | A | 429 | 17.069 | 13.526 | 68.414 | 1.00 | 29.53 |
| ATOM | 3395 | CD1 | TYR | A | 429 | 16.823 | 14.714 | 69.114 | 1.00 | 31.11 |
| ATOM | 3396 | CD2 | TYR | A | 429 | 17.361 | 12.383 | 69.156 | 1.00 | 32.70 |
| ATOM | 3397 | CE1 | TYR | A | 429 | 16.916 | 14.769 | 70.510 | 1.00 | 32.23 |
| ATOM | 3398 | CE2 | TYR | A | 429 | 17.485 | 12.420 | 70.551 | 1.00 | 35.30 |
| ATOM | 3399 | CZ  | TYR | A | 429 | 17.251 | 13.623 | 71.231 | 1.00 | 41.02 |
| ATOM | 3400 | OH  | TYR | A | 429 | 17.339 | 13.679 | 72.609 | 1.00 | 30.02 |
| ATOM | 3401 | N   | SER | A | 430 | 17.748 | 13.342 | 63.854 | 1.00 | 21.68 |
| ATOM | 3402 | CA  | SER | A | 430 | 17.914 | 12.469 | 62.730 | 1.00 | 23.42 |
| ATOM | 3403 | C   | SER | A | 430 | 19.264 | 12.722 | 62.050 | 1.00 | 32.87 |
| ATOM | 3404 | O   | SER | A | 430 | 19.879 | 11.819 | 61.467 | 1.00 | 35.11 |
| ATOM | 3405 | CB  | SER | A | 430 | 16.756 | 12.541 | 61.773 | 1.00 | 28.79 |
| ATOM | 3406 | OG  | SER | A | 430 | 17.089 | 13.475 | 60.777 | 1.00 | 49.56 |
| ATOM | 3407 | N   | TYR | A | 431 | 19.748 | 13.955 | 62.132 | 1.00 | 27.18 |
| ATOM | 3408 | CA  | TYR | A | 431 | 21.017 | 14.296 | 61.537 | 1.00 | 27.14 |
| ATOM | 3409 | C   | TYR | A | 431 | 22.152 | 13.702 | 62.316 | 1.00 | 32.52 |
| ATOM | 3410 | O   | TYR | A | 431 | 23.155 | 13.242 | 61.771 | 1.00 | 33.64 |
| ATOM | 3411 | CB  | TYR | A | 431 | 21.216 | 15.818 | 61.385 | 1.00 | 31.07 |
| ATOM | 3412 | CG  | TYR | A | 431 | 22.566 | 16.265 | 60.812 | 1.00 | 35.63 |
| ATOM | 3413 | CD1 | TYR | A | 431 | 23.663 | 16.492 | 61.650 | 1.00 | 36.88 |
| ATOM | 3414 | CD2 | TYR | A | 431 | 22.735 | 16.496 | 59.444 | 1.00 | 36.92 |
| ATOM | 3415 | CE1 | TYR | A | 431 | 24.894 | 16.924 | 61.157 | 1.00 | 33.78 |
| ATOM | 3416 | CE2 | TYR | A | 431 | 23.964 | 16.916 | 58.924 | 1.00 | 37.86 |
| ATOM | 3417 | CZ  | TYR | A | 431 | 25.038 | 17.143 | 59.786 | 1.00 | 46.01 |
| ATOM | 3418 | OH  | TYR | A | 431 | 26.247 | 17.573 | 59.294 | 1.00 | 51.28 |
| ATOM | 3419 | N   | PHE | A | 432 | 21.964 | 13.728 | 63.606 | 1.00 | 29.66 |
| ATOM | 3420 | CA  | PHE | A | 432 | 22.939 | 13.215 | 64.526 | 1.00 | 29.12 |
| ATOM | 3421 | C   | PHE | A | 432 | 22.522 | 11.865 | 65.007 | 1.00 | 42.64 |
| ATOM | 3422 | O   | PHE | A | 432 | 22.499 | 11.593 | 66.197 | 1.00 | 46.77 |
| ATOM | 3423 | CB  | PHE | A | 432 | 23.063 | 14.157 | 65.719 | 1.00 | 30.24 |
| ATOM | 3424 | CG  | PHE | A | 432 | 23.962 | 15.327 | 65.401 | 1.00 | 33.03 |



|      |      |     |     |   |     |        |        |        |      |        |
|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
| ATOM | 3425 | CD1 | PHE | A | 432 | 25.336 | 15.113 | 65.277 | 1.00 | 37.22  |
| ATOM | 3426 | CD2 | PHE | A | 432 | 23.470 | 16.624 | 65.232 | 1.00 | 30.70  |
| ATOM | 3427 | CE1 | PHE | A | 432 | 26.223 | 16.153 | 64.999 | 1.00 | 34.27  |
| ATOM | 3428 | CE2 | PHE | A | 432 | 24.349 | 17.667 | 64.938 | 1.00 | 31.71  |
| ATOM | 3429 | CZ  | PHE | A | 432 | 25.722 | 17.438 | 64.823 | 1.00 | 27.82  |
| ATOM | 3430 | N   | LYS | A | 433 | 22.174 | 11.029 | 64.063 | 1.00 | 42.50  |
| ATOM | 3431 | CA  | LYS | A | 433 | 21.669 | 9.670  | 64.270 | 1.00 | 40.87  |
| ATOM | 3432 | C   | LYS | A | 433 | 22.718 | 8.751  | 64.908 | 1.00 | 46.17  |
| ATOM | 3433 | O   | LYS | A | 433 | 22.405 | 7.734  | 65.513 | 1.00 | 48.48  |
| ATOM | 3434 | CB  | LYS | A | 433 | 21.245 | 9.106  | 62.917 | 1.00 | 39.25  |
| ATOM | 3435 | CG  | LYS | A | 433 | 19.988 | 8.241  | 63.017 | 1.00 | 84.17  |
| ATOM | 3436 | CD  | LYS | A | 433 | 18.925 | 8.660  | 62.000 | 1.00 | 100.00 |
| ATOM | 3437 | CE  | LYS | A | 433 | 17.523 | 8.172  | 62.384 | 1.00 | 100.00 |
| ATOM | 3438 | NZ  | LYS | A | 433 | 16.525 | 9.119  | 61.884 | 1.00 | 100.00 |
| ATOM | 3439 | N   | ASP | A | 434 | 24.002 | 9.112  | 64.697 | 1.00 | 45.20  |
| ATOM | 3440 | CA  | ASP | A | 434 | 25.083 | 8.349  | 65.321 | 1.00 | 47.80  |
| ATOM | 3441 | C   | ASP | A | 434 | 25.201 | 8.684  | 66.802 | 1.00 | 50.78  |
| ATOM | 3442 | O   | ASP | A | 434 | 25.474 | 7.845  | 67.653 | 1.00 | 55.76  |
| ATOM | 3443 | CB  | ASP | A | 434 | 26.405 | 8.567  | 64.562 | 1.00 | 53.91  |
| ATOM | 3444 | CG  | ASP | A | 434 | 26.123 | 8.474  | 63.069 | 1.00 | 93.32  |
| ATOM | 3445 | OD1 | ASP | A | 434 | 25.744 | 7.573  | 62.325 | 1.00 | 96.22  |
| ATOM | 3446 | OD2 | ASP | A | 434 | 26.119 | 9.664  | 62.753 | 1.00 | 100.00 |
| ATOM | 3447 | N   | LYS | A | 435 | 25.015 | 9.978  | 67.085 | 1.00 | 38.82  |
| ATOM | 3448 | CA  | LYS | A | 435 | 24.974 | 10.404 | 68.468 | 1.00 | 34.57  |
| ATOM | 3449 | C   | LYS | A | 435 | 23.549 | 10.749 | 68.881 | 1.00 | 39.87  |
| ATOM | 3450 | O   | LYS | A | 435 | 23.070 | 11.840 | 68.693 | 1.00 | 40.34  |
| ATOM | 3451 | CB  | LYS | A | 435 | 25.864 | 11.631 | 68.615 | 1.00 | 34.69  |
| ATOM | 3452 | CG  | LYS | A | 435 | 27.064 | 11.595 | 67.679 | 1.00 | 40.86  |
| ATOM | 3453 | CD  | LYS | A | 435 | 27.703 | 12.975 | 67.532 | 1.00 | 51.04  |
| ATOM | 3454 | CE  | LYS | A | 435 | 29.242 | 12.904 | 67.557 | 1.00 | 24.08  |
| ATOM | 3455 | NZ  | LYS | A | 435 | 29.822 | 13.990 | 66.760 | 1.00 | 45.26  |
| ATOM | 3456 | N   | VAL | A | 436 | 22.843 | 9.728  | 69.414 | 1.00 | 38.07  |
| ATOM | 3457 | CA  | VAL | A | 436 | 21.601 | 10.036 | 70.111 | 1.00 | 36.86  |
| ATOM | 3458 | C   | VAL | A | 436 | 21.846 | 10.129 | 71.608 | 1.00 | 44.88  |
| ATOM | 3459 | O   | VAL | A | 436 | 21.289 | 10.948 | 72.300 | 1.00 | 46.42  |
| ATOM | 3460 | CB  | VAL | A | 436 | 20.567 | 8.923  | 69.816 | 1.00 | 37.37  |
| ATOM | 3461 | CG1 | VAL | A | 436 | 19.944 | 9.143  | 68.446 | 1.00 | 36.24  |
| ATOM | 3462 | CG2 | VAL | A | 436 | 21.227 | 7.556  | 69.854 | 1.00 | 36.80  |
| ATOM | 3463 | N   | ASP | A | 437 | 22.718 | 9.232  | 72.099 | 1.00 | 43.61  |
| ATOM | 3464 | CA  | ASP | A | 437 | 23.044 | 9.222  | 73.522 | 1.00 | 41.43  |
| ATOM | 3465 | C   | ASP | A | 437 | 23.657 | 10.546 | 73.958 | 1.00 | 45.71  |
| ATOM | 3466 | O   | ASP | A | 437 | 23.554 | 10.956 | 75.107 | 1.00 | 49.89  |
| ATOM | 3467 | CB  | ASP | A | 437 | 24.022 | 8.082  | 73.776 | 1.00 | 43.84  |
| ATOM | 3468 | CG  | ASP | A | 437 | 23.281 | 6.752  | 73.691 | 1.00 | 72.47  |
| ATOM | 3469 | OD1 | ASP | A | 437 | 22.062 | 6.769  | 73.823 | 1.00 | 74.64  |
| ATOM | 3470 | OD2 | ASP | A | 437 | 23.933 | 5.730  | 73.481 | 1.00 | 86.09  |
| ATOM | 3471 | N   | VAL | A | 438 | 24.333 | 11.324 | 73.122 | 1.00 | 40.21  |
| ATOM | 3472 | CA  | VAL | A | 438 | 24.807 | 12.624 | 73.577 | 1.00 | 40.97  |
| ATOM | 3473 | C   | VAL | A | 438 | 23.621 | 13.582 | 73.668 | 1.00 | 41.86  |
| ATOM | 3474 | O   | VAL | A | 438 | 23.368 | 14.276 | 74.657 | 1.00 | 39.95  |
| ATOM | 3475 | CB  | VAL | A | 438 | 25.875 | 13.165 | 72.615 | 1.00 | 47.47  |
| ATOM | 3476 | CG1 | VAL | A | 438 | 26.438 | 14.523 | 73.051 | 1.00 | 47.51  |
| ATOM | 3477 | CG2 | VAL | A | 438 | 26.996 | 12.149 | 72.440 | 1.00 | 47.51  |
| ATOM | 3478 | N   | LEU | A | 439 | 22.876 | 13.595 | 72.585 | 1.00 | 37.91  |
| ATOM | 3479 | CA  | LEU | A | 439 | 21.729 | 14.442 | 72.507 | 1.00 | 36.21  |
| ATOM | 3480 | C   | LEU | A | 439 | 20.850 | 14.190 | 73.695 | 1.00 | 40.03  |
| ATOM | 3481 | O   | LEU | A | 439 | 20.214 | 15.064 | 74.255 | 1.00 | 42.22  |
| ATOM | 3482 | CB  | LEU | A | 439 | 20.949 | 14.180 | 71.210 | 1.00 | 33.84  |
| ATOM | 3483 | CG  | LEU | A | 439 | 21.552 | 14.939 | 70.039 | 1.00 | 32.80  |
| ATOM | 3484 | CD1 | LEU | A | 439 | 20.813 | 14.538 | 68.775 | 1.00 | 34.08  |
| ATOM | 3485 | CD2 | LEU | A | 439 | 21.435 | 16.434 | 70.258 | 1.00 | 23.80  |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 3486 | N   | ASN | A | 440 | 20.810 | 12.953 | 74.076 | 1.00 | 34.03 |
| ATOM | 3487 | CA  | ASN | A | 440 | 19.971 | 12.603 | 75.187 | 1.00 | 34.00 |
| ATOM | 3488 | C   | ASN | A | 440 | 20.494 | 13.093 | 76.532 | 1.00 | 40.95 |
| ATOM | 3489 | O   | ASN | A | 440 | 19.816 | 12.995 | 77.544 | 1.00 | 42.09 |
| ATOM | 3490 | CB  | ASN | A | 440 | 19.681 | 11.095 | 75.178 | 1.00 | 24.89 |
| ATOM | 3491 | CG  | ASN | A | 440 | 18.790 | 10.635 | 74.028 | 1.00 | 46.52 |
| ATOM | 3492 | OD1 | ASN | A | 440 | 19.005 | 9.537  | 73.480 | 1.00 | 58.82 |
| ATOM | 3493 | ND2 | ASN | A | 440 | 17.769 | 11.440 | 73.680 | 1.00 | 31.11 |
| ATOM | 3494 | N   | GLN | A | 441 | 21.707 | 13.623 | 76.531 | 1.00 | 36.98 |
| ATOM | 3495 | CA  | GLN | A | 441 | 22.339 | 14.095 | 77.744 | 1.00 | 35.47 |
| ATOM | 3496 | C   | GLN | A | 441 | 21.879 | 15.478 | 78.067 | 1.00 | 36.00 |
| ATOM | 3497 | O   | GLN | A | 441 | 22.137 | 16.029 | 79.142 | 1.00 | 34.96 |
| ATOM | 3498 | CB  | GLN | A | 441 | 23.878 | 14.109 | 77.581 | 1.00 | 38.10 |
| ATOM | 3499 | CG  | GLN | A | 441 | 24.504 | 12.692 | 77.422 | 1.00 | 52.06 |
| ATOM | 3500 | CD  | GLN | A | 441 | 25.954 | 12.730 | 76.955 | 1.00 | 81.69 |
| ATOM | 3501 | OE1 | GLN | A | 441 | 26.476 | 13.796 | 76.609 | 1.00 | 74.46 |
| ATOM | 3502 | NE2 | GLN | A | 441 | 26.616 | 11.574 | 76.972 | 1.00 | 91.09 |
| ATOM | 3503 | N   | VAL | A | 442 | 21.197 | 16.067 | 77.112 | 1.00 | 31.86 |
| ATOM | 3504 | CA  | VAL | A | 442 | 20.753 | 17.411 | 77.384 | 1.00 | 32.78 |
| ATOM | 3505 | C   | VAL | A | 442 | 19.354 | 17.468 | 77.970 | 1.00 | 38.24 |
| ATOM | 3506 | O   | VAL | A | 442 | 18.468 | 16.700 | 77.588 | 1.00 | 42.83 |
| ATOM | 3507 | CB  | VAL | A | 442 | 20.845 | 18.277 | 76.159 | 1.00 | 34.84 |
| ATOM | 3508 | CG1 | VAL | A | 442 | 21.430 | 17.435 | 75.020 | 1.00 | 34.65 |
| ATOM | 3509 | CG2 | VAL | A | 442 | 19.441 | 18.705 | 75.811 | 1.00 | 33.21 |
| ATOM | 3510 | N   | ASP | A | 443 | 19.172 | 18.388 | 78.908 | 1.00 | 25.60 |
| ATOM | 3511 | CA  | ASP | A | 443 | 17.931 | 18.634 | 79.616 | 1.00 | 24.57 |
| ATOM | 3512 | C   | ASP | A | 443 | 16.996 | 19.533 | 78.791 | 1.00 | 32.14 |
| ATOM | 3513 | O   | ASP | A | 443 | 16.744 | 20.732 | 79.073 | 1.00 | 34.77 |
| ATOM | 3514 | CB  | ASP | A | 443 | 18.332 | 19.272 | 80.957 | 1.00 | 27.11 |
| ATOM | 3515 | CG  | ASP | A | 443 | 17.216 | 19.413 | 81.901 | 1.00 | 39.99 |
| ATOM | 3516 | OD1 | ASP | A | 443 | 16.063 | 19.234 | 81.573 | 1.00 | 44.78 |
| ATOM | 3517 | OD2 | ASP | A | 443 | 17.631 | 19.753 | 83.094 | 1.00 | 56.66 |
| ATOM | 3518 | N   | TRP | A | 444 | 16.525 | 18.914 | 77.722 | 1.00 | 28.30 |
| ATOM | 3519 | CA  | TRP | A | 444 | 15.614 | 19.507 | 76.757 | 1.00 | 26.27 |
| ATOM | 3520 | C   | TRP | A | 444 | 14.460 | 20.296 | 77.416 | 1.00 | 31.52 |
| ATOM | 3521 | O   | TRP | A | 444 | 14.102 | 21.409 | 76.988 | 1.00 | 34.63 |
| ATOM | 3522 | CB  | TRP | A | 444 | 15.067 | 18.398 | 75.799 | 1.00 | 21.47 |
| ATOM | 3523 | CG  | TRP | A | 444 | 16.095 | 17.951 | 74.806 | 1.00 | 22.03 |
| ATOM | 3524 | CD1 | TRP | A | 444 | 16.675 | 16.718 | 74.736 | 1.00 | 25.16 |
| ATOM | 3525 | CD2 | TRP | A | 444 | 16.733 | 18.738 | 73.776 | 1.00 | 20.36 |
| ATOM | 3526 | NE1 | TRP | A | 444 | 17.623 | 16.677 | 73.738 | 1.00 | 23.97 |
| ATOM | 3527 | CE2 | TRP | A | 444 | 17.688 | 17.906 | 73.138 | 1.00 | 24.71 |
| ATOM | 3528 | CE3 | TRP | A | 444 | 1      |        |        |      |       |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 3547 | C   | TRP | A | 447 | 14.989 | 24.912 | 77.223 | 1.00 | 31.32 |
| ATOM | 3548 | O   | TRP | A | 447 | 14.971 | 26.089 | 76.875 | 1.00 | 30.48 |
| ATOM | 3549 | CB  | TRP | A | 447 | 17.166 | 23.725 | 77.062 | 1.00 | 25.78 |
| ATOM | 3550 | CG  | TRP | A | 447 | 18.625 | 23.815 | 77.421 | 1.00 | 26.60 |
| ATOM | 3551 | CD1 | TRP | A | 447 | 19.343 | 22.840 | 78.046 | 1.00 | 28.89 |
| ATOM | 3552 | CD2 | TRP | A | 447 | 19.554 | 24.896 | 77.165 | 1.00 | 26.16 |
| ATOM | 3553 | NE1 | TRP | A | 447 | 20.654 | 23.217 | 78.197 | 1.00 | 27.23 |
| ATOM | 3554 | CE2 | TRP | A | 447 | 20.822 | 24.476 | 77.660 | 1.00 | 29.00 |
| ATOM | 3555 | CE3 | TRP | A | 447 | 19.435 | 26.162 | 76.607 | 1.00 | 27.56 |
| ATOM | 3556 | CZ2 | TRP | A | 447 | 21.954 | 25.290 | 77.583 | 1.00 | 27.95 |
| ATOM | 3557 | CZ3 | TRP | A | 447 | 20.554 | 26.966 | 76.538 | 1.00 | 29.93 |
| ATOM | 3558 | CH2 | TRP | A | 447 | 21.792 | 26.539 | 77.035 | 1.00 | 30.16 |
| ATOM | 3559 | N   | LEU | A | 448 | 14.029 | 24.034 | 76.893 | 1.00 | 26.54 |
| ATOM | 3560 | CA  | LEU | A | 448 | 12.896 | 24.421 | 76.052 | 1.00 | 26.92 |
| ATOM | 3561 | C   | LEU | A | 448 | 11.734 | 25.064 | 76.779 | 1.00 | 36.15 |
| ATOM | 3562 | O   | LEU | A | 448 | 11.089 | 26.031 | 76.304 | 1.00 | 31.19 |
| ATOM | 3563 | CB  | LEU | A | 448 | 12.338 | 23.197 | 75.307 | 1.00 | 25.26 |
| ATOM | 3564 | CG  | LEU | A | 448 | 13.311 | 22.545 | 74.332 | 1.00 | 28.29 |
| ATOM | 3565 | CD1 | LEU | A | 448 | 12.597 | 21.455 | 73.530 | 1.00 | 30.49 |
| ATOM | 3566 | CD2 | LEU | A | 448 | 13.879 | 23.576 | 73.375 | 1.00 | 21.94 |
| ATOM | 3567 | N   | TYR | A | 449 | 11.472 | 24.455 | 77.924 | 1.00 | 33.14 |
| ATOM | 3568 | CA  | TYR | A | 449 | 10.373 | 24.835 | 78.747 | 1.00 | 30.64 |
| ATOM | 3569 | C   | TYR | A | 449 | 10.646 | 25.525 | 80.041 | 1.00 | 34.31 |
| ATOM | 3570 | O   | TYR | A | 449 | 9.750  | 26.191 | 80.529 | 1.00 | 41.98 |
| ATOM | 3571 | CB  | TYR | A | 449 | 9.400  | 23.674 | 78.916 | 1.00 | 29.14 |
| ATOM | 3572 | CG  | TYR | A | 449 | 9.212  | 23.089 | 77.556 | 1.00 | 26.50 |
| ATOM | 3573 | CD1 | TYR | A | 449 | 8.762  | 23.869 | 76.485 | 1.00 | 24.36 |
| ATOM | 3574 | CD2 | TYR | A | 449 | 9.560  | 21.762 | 77.325 | 1.00 | 28.48 |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 3575 | CE1 | TYR | A | 449 | 8.626  | 23.331 | 75.202 | 1.00 | 17.56 |
| ATOM | 3576 | CE2 | TYR | A | 449 | 9.427  | 21.205 | 76.054 | 1.00 | 29.93 |
| ATOM | 3577 | CZ  | TYR | A | 449 | 8.959  | 21.988 | 74.998 | 1.00 | 33.65 |
| ATOM | 3578 | OH  | TYR | A | 449 | 8.840  | 21.415 | 73.762 | 1.00 | 39.47 |
| ATOM | 3579 | N   | SER | A | 450 | 11.806 | 25.413 | 80.644 | 1.00 | 22.72 |
| ATOM | 3580 | CA  | SER | A | 450 | 11.902 | 26.149 | 81.900 | 1.00 | 21.21 |
| ATOM | 3581 | C   | SER | A | 450 | 12.278 | 27.625 | 81.749 | 1.00 | 23.98 |
| ATOM | 3582 | O   | SER | A | 450 | 12.966 | 28.035 | 80.810 | 1.00 | 27.17 |
| ATOM | 3583 | CB  | SER | A | 450 | 12.666 | 25.436 | 83.010 | 1.00 | 24.83 |
| ATOM | 3584 | OG  | SER | A | 450 | 12.540 | 24.046 | 82.871 | 1.00 | 36.29 |
| ATOM | 3585 | N   | PRO | A | 451 | 11.806 | 28.430 | 82.689 | 1.00 | 19.76 |
| ATOM | 3586 | CA  | PRO | A | 451 | 12.111 | 29.840 | 82.669 | 1.00 | 18.20 |
| ATOM | 3587 | C   | PRO | A | 451 | 13.461 | 29.988 | 83.271 | 1.00 | 21.72 |
| ATOM | 3588 | O   | PRO | A | 451 | 14.022 | 29.015 | 83.742 | 1.00 | 24.34 |
| ATOM | 3589 | CB  | PRO | A | 451 | 11.185 | 30.485 | 83.695 | 1.00 | 18.85 |
| ATOM | 3590 | CG  | PRO | A | 451 | 10.836 | 29.390 | 84.677 | 1.00 | 23.13 |
| ATOM | 3591 | CD  | PRO | A | 451 | 11.002 | 28.078 | 83.900 | 1.00 | 19.61 |
| ATOM | 3592 | N   | GLY | A | 452 | 13.959 | 31.212 | 83.307 | 1.00 | 18.97 |
| ATOM | 3593 | CA  | GLY | A | 452 | 15.241 | 31.444 | 83.922 | 1.00 | 19.09 |
| ATOM | 3594 | C   | GLY | A | 452 | 16.382 | 31.107 | 83.016 | 1.00 | 26.20 |
| ATOM | 3595 | O   | GLY | A | 452 | 16.191 | 30.916 | 81.819 | 1.00 | 27.37 |
| ATOM | 3596 | N   | LEU | A | 453 | 17.557 | 31.057 | 83.650 | 1.00 | 25.48 |
| ATOM | 3597 | CA  | LEU | A | 453 | 18.843 | 30.750 | 83.029 | 1.00 | 25.32 |
| ATOM | 3598 | C   | LEU | A | 453 | 18.906 | 29.322 | 82.629 | 1.00 | 26.21 |
| ATOM | 3599 | O   | LEU | A | 453 | 18.400 | 28.458 | 83.322 | 1.00 | 25.04 |
| ATOM | 3600 | CB  | LEU | A | 453 | 20.042 | 31.119 | 83.938 | 1.00 | 25.46 |
| ATOM | 3601 | CG  | LEU | A | 453 | 20.280 | 32.632 | 83.904 | 1.00 | 31.82 |
| ATOM | 3602 | CD1 | LEU | A | 453 | 21.019 | 33.087 | 85.119 | 1.00 | 31.78 |
| ATOM | 3603 | CD2 | LEU | A | 453 | 21.046 | 33.056 | 82.651 | 1.00 | 41.50 |
| ATOM | 3604 | N   | PRO | A | 454 | 19.510 | 29.082 | 81.489 | 1.00 | 22.97 |
| ATOM | 3605 | CA  | PRO | A | 454 | 19.585 | 27.747 | 81.003 | 1.00 | 21.60 |
| ATOM | 3606 | C   | PRO | A | 454 | 20.145 | 26.890 | 82.075 | 1.00 | 26.94 |
| ATOM | 3607 | O   | PRO | A | 454 | 20.923 | 27.359 | 82.893 | 1.00 | 29.09 |
| ATOM | 3608 | CB  | PRO | A | 454 | 20.489 | 27.780 | 79.768 | 1.00 | 22.34 |
| ATOM | 3609 | CG  | PRO | A | 454 | 20.777 | 29.232 | 79.470 | 1.00 | 23.69 |
| ATOM | 3610 | CD  | PRO | A | 454 | 20.136 | 30.054 | 80.556 | 1.00 | 20.82 |
| ATOM | 3611 | N   | PRO | A | 455 | 19.721 | 25.648 | 82.067 | 1.00 | 25.61 |
| ATOM | 3612 | CA  | PRO | A | 455 | 20.167 | 24.683 | 83.031 | 1.00 | 24.27 |
| ATOM | 3613 | C   | PRO | A | 455 | 21.661 | 24.568 | 82.991 | 1.00 | 30.95 |
| ATOM | 3614 | O   | PRO | A | 455 | 22.225 | 24.062 | 83.920 | 1.00 | 33.47 |
| ATOM | 3615 | CB  | PRO | A | 455 | 19.631 | 23.320 | 82.592 | 1.00 | 25.04 |
| ATOM | 3616 | CG  | PRO | A | 455 | 19.149 | 23.497 | 81.162 | 1.00 | 33.02 |
| ATOM | 3617 | CD  | PRO | A | 455 | 19.111 | 25.005 | 80.888 | 1.00 | 28.49 |
| ATOM | 3618 | N   | ILE | A | 456 | 22.305 | 25.002 | 81.911 | 1.00 | 27.91 |
| ATOM | 3619 | CA  | ILE | A | 456 | 23.764 | 24.893 | 81.821 | 1.00 | 27.82 |
| ATOM | 3620 | C   | ILE | A | 456 | 24.395 | 26.057 | 81.077 | 1.00 | 34.73 |
| ATOM | 3621 | O   | ILE | A | 456 | 23.737 | 26.769 | 80.293 | 1.00 | 37.01 |
| ATOM | 3622 | CB  | ILE | A | 456 | 24.228 | 23.540 | 81.259 | 1.00 | 31.34 |
| ATOM | 3623 | CG1 | ILE | A | 456 | 25.721 | 23.305 | 81.417 | 1.00 | 29.78 |
| ATOM | 3624 | CG2 | ILE | A | 456 | 23.865 | 23.369 | 79.788 | 1.00 | 32.96 |
| ATOM | 3625 | CD1 | ILE | A | 456 | 26.054 | 21.852 | 81.116 | 1.00 | 23.94 |
| ATOM | 3626 | N   | LYS | A | 457 | 25.680 | 26.252 | 81.334 | 1.00 | 30.52 |
| ATOM | 3627 | CA  | LYS | A | 457 | 26.405 | 27.335 | 80.707 | 1.00 | 30.21 |
| ATOM | 3628 | C   | LYS | A | 457 | 27.515 | 26.808 | 79.835 | 1.00 | 32.14 |
| ATOM | 3629 | O   | LYS | A | 457 | 28.328 | 26.037 | 80.273 | 1.00 | 33.07 |
| ATOM | 3630 | CB  | LYS | A | 457 | 26.953 | 28.264 | 81.749 | 1.00 | 32.38 |
| ATOM | 3631 | CG  | LYS | A | 457 | 27.818 | 29.327 | 81.121 | 1.00 | 34.64 |
| ATOM | 3632 | CD  | LYS | A | 457 | 28.288 | 30.306 | 82.166 | 1.00 | 13.41 |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 3633 | CE  | LYS | A | 457 | 28.803 | 31.596 | 81.565 | 1.00 | 18.04 |
| ATOM | 3634 | NZ  | LYS | A | 457 | 28.974 | 32.643 | 82.595 | 1.00 | 26.77 |
| ATOM | 3635 | N   | PRO | A | 458 | 27.567 | 27.208 | 78.589 | 1.00 | 27.50 |
| ATOM | 3636 | CA  | PRO | A | 458 | 28.630 | 26.675 | 77.737 | 1.00 | 26.85 |
| ATOM | 3637 | C   | PRO | A | 458 | 29.994 | 27.147 | 78.185 | 1.00 | 26.89 |
| ATOM | 3638 | O   | PRO | A | 458 | 30.128 | 27.876 | 79.167 | 1.00 | 24.86 |
| ATOM | 3639 | CB  | PRO | A | 458 | 28.335 | 27.191 | 76.316 | 1.00 | 29.41 |
| ATOM | 3640 | CG  | PRO | A | 458 | 26.952 | 27.864 | 76.375 | 1.00 | 33.24 |
| ATOM | 3641 | CD  | PRO | A | 458 | 26.574 | 28.044 | 77.848 | 1.00 | 26.12 |
| ATOM | 3642 | N   | ASN | A | 459 | 31.005 | 26.754 | 77.440 | 1.00 | 22.13 |
| ATOM | 3643 | CA  | ASN | A | 459 | 32.359 | 27.191 | 77.735 | 1.00 | 22.29 |
| ATOM | 3644 | C   | ASN | A | 459 | 32.751 | 28.325 | 76.820 | 1.00 | 30.27 |
| ATOM | 3645 | O   | ASN | A | 459 | 32.451 | 28.296 | 75.617 | 1.00 | 32.89 |
| ATOM | 3646 | CB  | ASN | A | 459 | 33.315 | 26.060 | 77.494 | 1.00 | 25.03 |
| ATOM | 3647 | CG  | ASN | A | 459 | 32.766 | 24.846 | 78.155 | 1.00 | 49.54 |
| ATOM | 3648 | OD1 | ASN | A | 459 | 32.618 | 24.822 | 79.383 | 1.00 | 50.09 |
| ATOM | 3649 | ND2 | ASN | A | 459 | 32.411 | 23.870 | 77.332 | 1.00 | 38.39 |
| ATOM | 3650 | N   | TYR | A | 460 | 33.448 | 29.316 | 77.380 | 1.00 | 25.58 |
| ATOM | 3651 | CA  | TYR | A | 460 | 33.851 | 30.493 | 76.625 | 1.00 | 23.89 |
| ATOM | 3652 | C   | TYR | A | 460 | 35.298 | 30.853 | 76.745 | 1.00 | 34.20 |
| ATOM | 3653 | O   | TYR | A | 460 | 35.849 | 30.862 | 77.839 | 1.00 | 35.27 |
| ATOM | 3654 | CB  | TYR | A | 460 | 33.120 | 31.708 | 77.171 | 1.00 | 24.38 |
| ATOM | 3655 | CG  | TYR | A | 460 | 31.636 | 31.631 | 77.024 | 1.00 | 26.98 |
| ATOM | 3656 | CD1 | TYR | A | 460 | 31.029 | 32.011 | 75.829 | 1.00 | 30.69 |
| ATOM | 3657 | CD2 | TYR | A | 460 | 30.838 | 31.168 | 78.064 | 1.00 | 25.70 |
| ATOM | 3658 | CE1 | TYR | A | 460 | 29.644 | 31.952 | 75.684 | 1.00 | 28.77 |
| ATOM | 3659 | CE2 | TYR | A | 460 | 29.453 | 31.096 | 77.938 | 1.00 | 25.24 |
| ATOM | 3660 | CZ  | TYR | A | 460 | 28.863 | 31.496 | 76.741 | 1.00 | 24.49 |
| ATOM | 3661 | OH  | TYR | A | 460 | 27.519 | 31.443 | 76.587 | 1.00 | 28.39 |
| ATOM | 3662 | N   | ASP | A | 461 | 35.893 | 31.227 | 75.616 | 1.00 | 30.58 |
| ATOM | 3663 | CA  | ASP | A | 461 | 37.268 | 31.640 | 75.654 | 1.00 | 27.51 |
| ATOM | 3664 | C   | ASP | A | 461 | 37.319 | 32.941 | 76.464 | 1.00 | 23.53 |
| ATOM | 3665 | O   | ASP | A | 461 | 36.377 | 33.704 | 76.396 | 1.00 | 26.62 |
| ATOM | 3666 | CB  | ASP | A | 461 | 37.821 | 31.784 | 74.218 | 1.00 | 27.30 |
| ATOM | 3667 | CG  | ASP | A | 461 | 39.137 | 32.466 | 74.260 | 1.00 | 32.53 |
| ATOM | 3668 | OD1 | ASP | A | 461 | 39.262 | 33.672 | 74.334 | 1.00 | 39.66 |
| ATOM | 3669 | OD2 | ASP | A | 461 | 40.130 | 31.628 | 74.306 | 1.00 | 44.34 |
| ATOM | 3670 | N   | MET | A | 462 | 38.375 | 33.234 | 77.224 | 1.00 | 17.26 |
| ATOM | 3671 | CA  | MET | A | 462 | 38.396 | 34.511 | 78.008 | 1.00 | 18.66 |
| ATOM | 3672 | C   | MET | A | 462 | 39.299 | 35.634 | 77.485 | 1.00 | 24.02 |
| ATOM | 3673 | O   | MET | A | 462 | 39.336 | 36.738 | 78.011 | 1.00 | 24.56 |
| ATOM | 3674 | CB  | MET | A | 462 | 38.818 | 34.186 | 79.431 | 1.00 | 22.99 |
| ATOM | 3675 | CG  | MET | A | 462 | 37.808 |        |        |      |       |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 3691 | CD1 | LEU | A | 464 | 38.609 | 39.565 | 71.217 | 1.00 | 32.72 |
| ATOM | 3692 | CD2 | LEU | A | 464 | 40.648 | 40.261 | 72.499 | 1.00 | 26.22 |
| ATOM | 3693 | N   | THR | A | 465 | 37.855 | 39.167 | 76.964 | 1.00 | 30.71 |
| ATOM | 3694 | CA  | THR | A | 465 | 37.005 | 39.496 | 78.103 | 1.00 | 28.58 |
| ATOM | 3695 | C   | THR | A | 465 | 37.800 | 39.893 | 79.324 | 1.00 | 30.69 |
| ATOM | 3696 | O   | THR | A | 465 | 37.530 | 40.865 | 80.030 | 1.00 | 31.27 |
| ATOM | 3697 | CB  | THR | A | 465 | 36.016 | 38.328 | 78.372 | 1.00 | 35.85 |
| ATOM | 3698 | OG1 | THR | A | 465 | 35.101 | 38.212 | 77.296 | 1.00 | 50.93 |
| ATOM | 3699 | CG2 | THR | A | 465 | 35.255 | 38.451 | 79.690 | 1.00 | 26.34 |
| ATOM | 3700 | N   | ASN | A | 466 | 38.802 | 39.111 | 79.568 | 1.00 | 24.40 |
| ATOM | 3701 | CA  | ASN | A | 466 | 39.635 | 39.375 | 80.688 | 1.00 | 23.11 |
| ATOM | 3702 | C   | ASN | A | 466 | 39.899 | 40.856 | 80.967 | 1.00 | 28.37 |
| ATOM | 3703 | O   | ASN | A | 466 | 39.763 | 41.270 | 82.120 | 1.00 | 27.03 |
| ATOM | 3704 | CB  | ASN | A | 466 | 40.921 | 38.543 | 80.629 | 1.00 | 20.30 |
| ATOM | 3705 | CG  | ASN | A | 466 | 40.709 | 37.145 | 81.155 | 1.00 | 32.26 |
| ATOM | 3706 | OD1 | ASN | A | 466 | 41.384 | 36.191 | 80.723 | 1.00 | 29.29 |
| ATOM | 3707 | ND2 | ASN | A | 466 | 39.775 | 37.015 | 82.111 | 1.00 | 28.19 |
| ATOM | 3708 | N   | ALA | A | 467 | 40.306 | 41.666 | 79.967 | 1.00 | 27.97 |
| ATOM | 3709 | CA  | ALA | A | 467 | 40.587 | 43.079 | 80.295 | 1.00 | 26.66 |
| ATOM | 3710 | C   | ALA | A | 467 | 39.352 | 43.827 | 80.720 | 1.00 | 31.78 |
| ATOM | 3711 | O   | ALA | A | 467 | 39.406 | 44.845 | 81.393 | 1.00 | 31.71 |
| ATOM | 3712 | CB  | ALA | A | 467 | 41.365 | 43.837 | 79.256 | 1.00 | 25.99 |
| ATOM | 3713 | N   | CYS | A | 468 | 38.217 | 43.277 | 80.336 | 1.00 | 28.06 |
| ATOM | 3714 | CA  | CYS | A | 468 | 36.942 | 43.862 | 80.693 | 1.00 | 25.80 |
| ATOM | 3715 | C   | CYS | A | 468 | 36.668 | 43.619 | 82.165 | 1.00 | 26.47 |
| ATOM | 3716 | O   | CYS | A | 468 | 36.469 | 44.517 | 82.963 | 1.00 | 27.99 |
| ATOM | 3717 | CB  | CYS | A | 468 | 35.882 | 43.376 | 79.696 | 1.00 | 24.56 |
| ATOM | 3718 | SG  | CYS | A | 468 | 36.455 | 43.873 | 78.049 | 1.00 | 27.76 |
| ATOM | 3719 | N   | ILE | A | 469 | 36.752 | 42.384 | 82.540 | 1.00 | 24.34 |
| ATOM | 3720 | CA  | ILE | A | 469 | 36.599 | 42.052 | 83.921 | 1.00 | 25.23 |
| ATOM | 3721 | C   | ILE | A | 469 | 37.560 | 42.800 | 84.876 | 1.00 | 28.13 |
| ATOM | 3722 | O   | ILE | A | 469 | 37.175 | 43.220 | 85.950 | 1.00 | 29.54 |
| ATOM | 3723 | CB  | ILE | A | 469 | 36.858 | 40.574 | 84.068 | 1.00 | 27.23 |
| ATOM | 3724 | CG1 | ILE | A | 469 | 35.956 | 39.801 | 83.112 | 1.00 | 26.94 |
| ATOM | 3725 | CG2 | ILE | A | 469 | 36.537 | 40.208 | 85.496 | 1.00 | 25.56 |
| ATOM | 3726 | CD1 | ILE | A | 469 | 36.247 | 38.298 | 83.085 | 1.00 | 45.50 |
| ATOM | 3727 | N   | ALA | A | 470 | 38.830 | 42.960 | 84.534 | 1.00 | 23.28 |
| ATOM | 3728 | CA  | ALA | A | 470 | 39.749 | 43.621 | 85.461 | 1.00 | 22.23 |
| ATOM | 3729 | C   | ALA | A | 470 | 39.392 | 45.038 | 85.808 | 1.00 | 30.29 |
| ATOM | 3730 | O   | ALA | A | 470 | 39.474 | 45.451 | 86.986 | 1.00 | 32.82 |
| ATOM | 3731 | CB  | ALA | A | 470 | 41.218 | 43.502 | 85.074 | 1.00 | 21.98 |
| ATOM | 3732 | N   | LEU | A | 471 | 39.007 | 45.760 | 84.759 | 1.00 | 23.53 |
| ATOM | 3733 | CA  | LEU | A | 471 | 38.643 | 47.173 | 84.834 | 1.00 | 18.39 |
| ATOM | 3734 | C   | LEU | A | 471 | 37.333 | 47.373 | 85.569 | 1.00 | 26.57 |
| ATOM | 3735 | O   | LEU | A | 471 | 37.210 | 48.208 | 86.462 | 1.00 | 30.48 |
| ATOM | 3736 | CB  | LEU | A | 471 | 38.676 | 47.827 | 83.444 | 1.00 | 15.51 |
| ATOM | 3737 | CG  | LEU | A | 471 | 38.671 | 49.325 | 83.539 | 1.00 | 24.20 |
| ATOM | 3738 | CD1 | LEU | A | 471 | 39.754 | 49.795 | 84.513 | 1.00 | 24.86 |
| ATOM | 3739 | CD2 | LEU | A | 471 | 38.876 | 49.941 | 82.156 | 1.00 | 26.35 |
| ATOM | 3740 | N   | SER | A | 472 | 36.351 | 46.570 | 85.222 | 1.00 | 25.31 |
| ATOM | 3741 | CA  | SER | A | 472 | 35.080 | 46.674 | 85.901 | 1.00 | 27.56 |
| ATOM | 3742 | C   | SER | A | 472 | 35.260 | 46.477 | 87.396 | 1.00 | 33.46 |
| ATOM | 3743 | O   | SER | A | 472 | 34.800 | 47.292 | 88.214 | 1.00 | 32.85 |
| ATOM | 3744 | CB  | SER | A | 472 | 33.989 | 45.714 | 85.393 | 1.00 | 32.06 |
| ATOM | 3745 | OG  | SER | A | 472 | 34.492 | 44.774 | 84.470 | 1.00 | 48.56 |
| ATOM | 3746 | N   | GLN | A | 473 | 35.911 | 45.350 | 87.736 | 1.00 | 27.52 |
| ATOM | 3747 | CA  | GLN | A | 473 | 36.170 | 44.971 | 89.108 | 1.00 | 24.10 |
| ATOM | 3748 | C   | GLN | A | 473 | 36.866 | 46.096 | 89.836 | 1.00 | 25.18 |



009220-0122409

|      |      |     |     |   |     |        |        |         |      |       |
|------|------|-----|-----|---|-----|--------|--------|---------|------|-------|
| ATOM | 3749 | O   | GLN | A | 473 | 36.534 | 46.458 | 90.969  | 1.00 | 21.62 |
| ATOM | 3750 | CB  | GLN | A | 473 | 36.994 | 43.671 | 89.148  | 1.00 | 25.86 |
| ATOM | 3751 | CG  | GLN | A | 473 | 36.128 | 42.402 | 89.118  | 1.00 | 32.72 |
| ATOM | 3752 | CD  | GLN | A | 473 | 34.970 | 42.504 | 90.090  | 1.00 | 46.08 |
| ATOM | 3753 | OE1 | GLN | A | 473 | 35.165 | 42.422 | 91.308  | 1.00 | 40.73 |
| ATOM | 3754 | NE2 | GLN | A | 473 | 33.761 | 42.692 | 89.559  | 1.00 | 28.28 |
| ATOM | 3755 | N   | ARG | A | 474 | 37.855 | 46.656 | 89.161  | 1.00 | 24.00 |
| ATOM | 3756 | CA  | ARG | A | 474 | 38.562 | 47.765 | 89.779  | 1.00 | 24.46 |
| ATOM | 3757 | C   | ARG | A | 474 | 37.609 | 48.893 | 90.141  | 1.00 | 29.31 |
| ATOM | 3758 | O   | ARG | A | 474 | 37.620 | 49.447 | 91.242  | 1.00 | 33.13 |
| ATOM | 3759 | CB  | ARG | A | 474 | 39.682 | 48.290 | 88.898  | 1.00 | 20.19 |
| ATOM | 3760 | CG  | ARG | A | 474 | 40.866 | 47.352 | 88.831  | 1.00 | 28.48 |
| ATOM | 3761 | CD  | ARG | A | 474 | 41.871 | 47.869 | 87.832  | 1.00 | 34.41 |
| ATOM | 3762 | NE  | ARG | A | 474 | 42.258 | 49.245 | 88.093  | 1.00 | 40.09 |
| ATOM | 3763 | CZ  | ARG | A | 474 | 42.927 | 49.938 | 87.185  | 1.00 | 51.25 |
| ATOM | 3764 | NH1 | ARG | A | 474 | 43.220 | 49.376 | 86.019  | 1.00 | 24.79 |
| ATOM | 3765 | NH2 | ARG | A | 474 | 43.316 | 51.199 | 87.444  | 1.00 | 20.43 |
| ATOM | 3766 | N   | TRP | A | 475 | 36.791 | 49.259 | 89.178  | 1.00 | 25.32 |
| ATOM | 3767 | CA  | TRP | A | 475 | 35.862 | 50.332 | 89.400  | 1.00 | 26.77 |
| ATOM | 3768 | C   | TRP | A | 475 | 34.881 | 49.962 | 90.474  | 1.00 | 27.52 |
| ATOM | 3769 | O   | TRP | A | 475 | 34.749 | 50.633 | 91.475  | 1.00 | 29.64 |
| ATOM | 3770 | CB  | TRP | A | 475 | 35.199 | 50.804 | 88.093  | 1.00 | 27.95 |
| ATOM | 3771 | CG  | TRP | A | 475 | 36.047 | 51.819 | 87.361  | 1.00 | 32.11 |
| ATOM | 3772 | CD1 | TRP | A | 475 | 36.873 | 51.592 | 86.298  | 1.00 | 35.65 |
| ATOM | 3773 | CD2 | TRP | A | 475 | 36.161 | 53.217 | 87.648  | 1.00 | 31.62 |
| ATOM | 3774 | NE1 | TRP | A | 475 | 37.484 | 52.748 | 85.904  | 1.00 | 34.92 |
| ATOM | 3775 | CE2 | TRP | A | 475 | 37.054 | 53.763 | 86.707  | 1.00 | 36.16 |
| ATOM | 3776 | CE3 | TRP | A | 475 | 35.588 | 54.040 | 88.606  | 1.00 | 32.63 |
| ATOM | 3777 | CZ2 | TRP | A | 475 | 37.372 | 55.112 | 86.719  | 1.00 | 36.24 |
| ATOM | 3778 | CZ3 | TRP | A | 475 | 35.897 | 55.375 | 88.616  | 1.00 | 34.74 |
| ATOM | 3779 | CH2 | TRP | A | 475 | 36.777 | 55.901 | 87.685  | 1.00 | 35.77 |
| ATOM | 3780 | N   | ILE | A | 476 | 34.234 | 48.847 | 90.279  | 1.00 | 26.36 |
| ATOM | 3781 | CA  | ILE | A | 476 | 33.268 | 48.386 | 91.235  | 1.00 | 28.33 |
| ATOM | 3782 | C   | ILE | A | 476 | 33.771 | 48.315 | 92.681  | 1.00 | 34.20 |
| ATOM | 3783 | O   | ILE | A | 476 | 33.056 | 48.595 | 93.637  | 1.00 | 36.89 |
| ATOM | 3784 | CB  | ILE | A | 476 | 32.722 | 47.070 | 90.761  | 1.00 | 32.23 |
| ATOM | 3785 | CG1 | ILE | A | 476 | 31.993 | 47.308 | 89.443  | 1.00 | 30.49 |
| ATOM | 3786 | CG2 | ILE | A | 476 | 31.864 | 46.376 | 91.851  | 1.00 | 34.86 |
| ATOM | 3787 | CD1 | ILE | A | 476 | 31.595 | 46.005 | 88.756  | 1.00 | 33.04 |
| ATOM | 3788 | N   | THR | A | 477 | 35.010 | 47.934 | 92.860  | 1.00 | 27.27 |
| ATOM | 3789 | CA  | THR | A | 477 | 35.558 | 47.846 | 94.194  | 1.00 | 24.15 |
| ATOM | 3790 | C   | THR | A | 477 | 36.416 | 49.052 | 94.523  | 1.00 | 27.30 |
| ATOM | 3791 | O   | THR | A | 477 | 37.120 | 49.065 | 95.519  | 1.00 | 27.36 |
| ATOM | 3792 | CB  | THR | A | 477 | 36.402 | 46.578 | 94.257  | 1.00 | 32.13 |
| ATOM | 3793 | OG1 | THR | A | 477 | 37.593 | 46.848 | 93.557  | 1.00 | 29.48 |
| ATOM | 3794 | CG2 | THR | A | 477 | 35.634 | 45.470 | 93.530  | 1.00 | 16.94 |
| ATOM | 3795 | N   | ALA | A | 478 | 36.371 | 50.097 | 93.695  | 1.00 | 22.33 |
| ATOM | 3796 | CA  | ALA | A | 478 | 37.164 | 51.260 | 93.988  | 1.00 | 20.44 |
| ATOM | 3797 | C   | ALA | A | 478 | 36.890 | 51.843 | 95.390  | 1.00 | 32.94 |
| ATOM | 3798 | O   | ALA | A | 478 | 35.786 | 51.756 | 95.922  | 1.00 | 34.38 |
| ATOM | 3799 | CB  | ALA | A | 478 | 36.938 | 52.343 | 92.942  | 1.00 | 19.26 |
| ATOM | 3800 | N   | LYS | A | 479 | 37.931 | 52.469 | 95.970  | 1.00 | 29.65 |
| ATOM | 3801 | CA  | LYS | A | 479 | 37.899 | 53.168 | 97.243  | 1.00 | 27.30 |
| ATOM | 3802 | C   | LYS | A | 479 | 38.575 | 54.512 | 97.051  | 1.00 | 36.54 |
| ATOM | 3803 | O   | LYS | A | 479 | 39.378 | 54.692 | 96.118  | 1.00 | 34.13 |
| ATOM | 3804 | CB  | LYS | A | 479 | 38.457 | 52.410 | 98.417  | 1.00 | 28.01 |
| ATOM | 3805 | CG  | LYS | A | 479 | 37.696 | 51.116 | 98.631  | 1.00 | 51.38 |
| ATOM | 3806 | CD  | LYS | A | 479 | 37.115 | 50.880 | 100.021 | 1.00 | 67.24 |



|      |      |     |     |   |     |        |        |         |      |        |
|------|------|-----|-----|---|-----|--------|--------|---------|------|--------|
| ATOM | 3807 | CE  | LYS | A | 479 | 35.804 | 50.103 | 99.931  | 1.00 | 87.12  |
| ATOM | 3808 | NZ  | LYS | A | 479 | 35.711 | 48.948 | 100.841 | 1.00 | 85.55  |
| ATOM | 3809 | N   | GLU | A | 480 | 38.241 | 55.477 | 97.900  | 1.00 | 36.30  |
| ATOM | 3810 | CA  | GLU | A | 480 | 38.843 | 56.793 | 97.751  | 1.00 | 34.79  |
| ATOM | 3811 | C   | GLU | A | 480 | 40.261 | 56.707 | 97.220  | 1.00 | 34.79  |
| ATOM | 3812 | O   | GLU | A | 480 | 40.613 | 57.332 | 96.234  | 1.00 | 34.10  |
| ATOM | 3813 | CB  | GLU | A | 480 | 38.899 | 57.565 | 99.078  | 1.00 | 36.21  |
| ATOM | 3814 | CG  | GLU | A | 480 | 37.709 | 58.500 | 99.303  | 1.00 | 63.85  |
| ATOM | 3815 | CD  | GLU | A | 480 | 37.601 | 59.511 | 98.214  | 1.00 | 100.00 |
| ATOM | 3816 | OE1 | GLU | A | 480 | 38.457 | 59.648 | 97.357  | 1.00 | 100.00 |
| ATOM | 3817 | OE2 | GLU | A | 480 | 36.491 | 60.209 | 98.288  | 1.00 | 100.00 |
| ATOM | 3818 | N   | ASP | A | 481 | 41.080 | 55.946 | 97.904  | 1.00 | 24.69  |
| ATOM | 3819 | CA  | ASP | A | 481 | 42.451 | 55.860 | 97.519  | 1.00 | 23.87  |
| ATOM | 3820 | C   | ASP | A | 481 | 42.771 | 55.314 | 96.132  | 1.00 | 34.51  |
| ATOM | 3821 | O   | ASP | A | 481 | 43.925 | 55.312 | 95.721  | 1.00 | 39.44  |
| ATOM | 3822 | CB  | ASP | A | 481 | 43.262 | 55.155 | 98.611  | 1.00 | 25.29  |
| ATOM | 3823 | CG  | ASP | A | 481 | 43.072 | 53.668 | 98.575  | 1.00 | 39.58  |
| ATOM | 3824 | OD1 | ASP | A | 481 | 42.471 | 53.029 | 97.708  | 1.00 | 46.00  |
| ATOM | 3825 | OD2 | ASP | A | 481 | 43.698 | 53.107 | 99.567  | 1.00 | 39.59  |
| ATOM | 3826 | N   | ASP | A | 482 | 41.788 | 54.881 | 95.373  | 1.00 | 30.70  |
| ATOM | 3827 | CA  | ASP | A | 482 | 42.098 | 54.379 | 94.024  | 1.00 | 31.73  |
| ATOM | 3828 | C   | ASP | A | 482 | 41.725 | 55.307 | 92.859  | 1.00 | 34.17  |
| ATOM | 3829 | O   | ASP | A | 482 | 42.158 | 55.150 | 91.717  | 1.00 | 35.45  |
| ATOM | 3830 | CB  | ASP | A | 482 | 41.399 | 53.022 | 93.756  | 1.00 | 33.31  |
| ATOM | 3831 | CG  | ASP | A | 482 | 41.686 | 51.970 | 94.779  | 1.00 | 38.90  |
| ATOM | 3832 | OD1 | ASP | A | 482 | 42.810 | 51.514 | 94.992  | 1.00 | 42.45  |
| ATOM | 3833 | OD2 | ASP | A | 482 | 40.606 | 51.625 | 95.440  | 1.00 | 40.17  |
| ATOM | 3834 | N   | LEU | A | 483 | 40.863 | 56.246 | 93.146  | 1.00 | 29.93  |
| ATOM | 3835 | CA  | LEU | A | 483 | 40.352 | 57.159 | 92.160  | 1.00 | 27.80  |
| ATOM | 3836 | C   | LEU | A | 483 | 41.434 | 57.943 | 91.410  | 1.00 | 40.70  |
| ATOM | 3837 | O   | LEU | A | 483 | 41.386 | 58.102 | 90.180  | 1.00 | 40.76  |
| ATOM | 3838 | CB  | LEU | A | 483 | 39.265 | 58.049 | 92.819  | 1.00 | 22.54  |
| ATOM | 3839 | CG  | LEU | A | 483 | 38.148 | 57.240 | 93.488  | 1.00 | 20.75  |
| ATOM | 3840 | CD1 | LEU | A | 483 | 37.170 | 58.165 | 94.197  | 1.00 | 19.29  |
| ATOM | 3841 | CD2 | LEU | A | 483 | 37.389 | 56.467 | 92.414  | 1.00 | 21.46  |
| ATOM | 3842 | N   | ASN | A | 484 | 42.410 | 58.446 | 92.162  | 1.00 | 36.15  |
| ATOM | 3843 | CA  | ASN | A | 484 | 43.459 | 59.225 | 91.571  | 1.00 | 34.08  |
| ATOM | 3844 | C   | ASN | A | 484 | 44.168 | 58.524 | 90.429  | 1.00 | 39.51  |
| ATOM | 3845 | O   | ASN | A | 484 | 44.456 | 59.091 | 89.359  | 1.00 | 38.59  |
| ATOM | 3846 | CB  | ASN | A | 484 | 44.495 | 59.602 | 92.618  | 1.00 | 34.26  |
| ATOM | 3847 | CG  | ASN | A | 484 | 45.807 | 59.955 | 91.941  | 1.00 | 100.00 |
| ATOM | 3848 | OD1 | ASN | A | 484 | 45.878 | 60.940 | 91.171  | 1.00 | 100.00 |
| ATOM | 3849 | ND2 | ASN | A | 484 | 46.836 | 59.134 | 92.186  | 1.00 | 100.00 |
| ATOM | 3850 | N   | SER | A | 485 | 44.472 | 57.268 | 90.698  | 1.00 | 35.37  |
| ATOM | 3851 | CA  | SER | A | 485 | 45.202 | 56.417 | 89.791  | 1.00 | 32.79  |
| ATOM | 3852 | C   | SER | A | 485 | 44.522 | 56.140 | 88.484  | 1.00 | 32.26  |
| ATOM | 3853 | O   | SER | A | 485 | 45.159 | 55.925 | 87.463  | 1.00 | 32.44  |
| ATOM | 3854 | CB  | SER | A | 485 | 45.565 | 55.132 | 90.477  | 1.00 | 38.65  |
| ATOM | 3855 | OG  | SER | A | 485 | 46.040 | 55.437 | 91.777  | 1.00 | 62.66  |
| ATOM | 3856 | N   | PHE | A | 486 | 43.222 | 56.110 | 88.491  | 1.00 | 27.13  |
| ATOM | 3857 | CA  | PHE | A | 486 | 42.631 | 55.809 | 87.233  | 1.00 | 28.26  |
| ATOM | 3858 | C   | PHE | A | 486 | 43.193 | 56.772 | 86.264  | 1.00 | 32.12  |
| ATOM | 3859 | O   | PHE | A | 486 | 43.423 | 57.910 | 86.604  | 1.00 | 32.02  |
| ATOM | 3860 | CB  | PHE | A | 486 | 41.101 | 55.819 | 87.198  | 1.00 | 31.01  |
| ATOM | 3861 | CG  | PHE | A | 486 | 40.471 | 54.807 | 88.132  | 1.00 | 27.04  |
| ATOM | 3862 | CD1 | PHE | A | 486 | 40.504 | 53.425 | 87.911  | 1.00 | 22.43  |
| ATOM | 3863 | CD2 | PHE | A | 486 | 39.805 | 55.293 | 89.253  | 1.00 | 21.40  |
| ATOM | 3864 | CE1 | PHE | A | 486 | 39.896 | 52.538 | 88.804  | 1.00 | 19.69  |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 3865 | CE2 | PHE | A | 486 | 39.224 | 54.426 | 90.174 | 1.00 | 19.20 |
| ATOM | 3866 | CZ  | PHE | A | 486 | 39.245 | 53.051 | 89.927 | 1.00 | 15.13 |
| ATOM | 3867 | N   | ASN | A | 487 | 43.455 | 56.279 | 85.089 | 1.00 | 34.97 |
| ATOM | 3868 | CA  | ASN | A | 487 | 44.032 | 57.092 | 84.070 | 1.00 | 38.06 |
| ATOM | 3869 | C   | ASN | A | 487 | 43.491 | 56.622 | 82.758 | 1.00 | 43.55 |
| ATOM | 3870 | O   | ASN | A | 487 | 42.951 | 55.537 | 82.604 | 1.00 | 46.30 |
| ATOM | 3871 | CB  | ASN | A | 487 | 45.591 | 57.038 | 84.085 | 1.00 | 43.93 |
| ATOM | 3872 | CG  | ASN | A | 487 | 46.196 | 58.169 | 83.302 | 1.00 | 56.10 |
| ATOM | 3873 | OD1 | ASN | A | 487 | 46.057 | 58.189 | 82.077 | 1.00 | 42.12 |
| ATOM | 3874 | ND2 | ASN | A | 487 | 46.829 | 59.112 | 84.007 | 1.00 | 65.62 |
| ATOM | 3875 | N   | ALA | A | 488 | 43.662 | 57.435 | 81.781 | 1.00 | 39.34 |
| ATOM | 3876 | CA  | ALA | A | 488 | 43.201 | 57.055 | 80.472 | 1.00 | 38.25 |
| ATOM | 3877 | C   | ALA | A | 488 | 44.024 | 55.900 | 79.809 | 1.00 | 43.58 |
| ATOM | 3878 | O   | ALA | A | 488 | 43.596 | 55.317 | 78.834 | 1.00 | 44.11 |
| ATOM | 3879 | CB  | ALA | A | 488 | 43.153 | 58.314 | 79.621 | 1.00 | 37.54 |
| ATOM | 3880 | N   | THR | A | 489 | 45.207 | 55.555 | 80.314 | 1.00 | 38.34 |
| ATOM | 3881 | CA  | THR | A | 489 | 45.996 | 54.499 | 79.715 | 1.00 | 36.16 |
| ATOM | 3882 | C   | THR | A | 489 | 45.270 | 53.181 | 79.792 | 1.00 | 45.74 |
| ATOM | 3883 | O   | THR | A | 489 | 45.476 | 52.233 | 79.057 | 1.00 | 47.78 |
| ATOM | 3884 | CB  | THR | A | 489 | 47.296 | 54.458 | 80.503 | 1.00 | 31.01 |
| ATOM | 3885 | OG1 | THR | A | 489 | 46.961 | 54.457 | 81.872 | 1.00 | 35.33 |
| ATOM | 3886 | CG2 | THR | A | 489 | 47.993 | 55.771 | 80.229 | 1.00 | 28.28 |
| ATOM | 3887 | N   | ASP | A | 490 | 44.337 | 53.182 | 80.708 | 1.00 | 46.75 |
| ATOM | 3888 | CA  | ASP | A | 490 | 43.560 | 52.018 | 80.972 | 1.00 | 51.49 |
| ATOM | 3889 | C   | ASP | A | 490 | 42.759 | 51.515 | 79.786 | 1.00 | 52.21 |
| ATOM | 3890 | O   | ASP | A | 490 | 42.396 | 50.342 | 79.651 | 1.00 | 54.75 |
| ATOM | 3891 | CB  | ASP | A | 490 | 42.676 | 52.345 | 82.184 | 1.00 | 54.04 |
| ATOM | 3892 | CG  | ASP | A | 490 | 43.413 | 52.884 | 83.380 | 1.00 | 53.83 |
| ATOM | 3893 | OD1 | ASP | A | 490 | 44.621 | 52.777 | 83.616 | 1.00 | 62.93 |
| ATOM | 3894 | OD2 | ASP | A | 490 | 42.565 | 53.446 | 84.165 | 1.00 | 35.66 |
| ATOM | 3895 | N   | LEU | A | 491 | 42.486 | 52.450 | 78.938 | 1.00 | 42.42 |
| ATOM | 3896 | CA  | LEU | A | 491 | 41.752 | 52.250 | 77.723 | 1.00 | 43.54 |
| ATOM | 3897 | C   | LEU | A | 491 | 42.712 | 51.977 | 76.585 | 1.00 | 43.97 |
| ATOM | 3898 | O   | LEU | A | 491 | 42.340 | 51.438 | 75.588 | 1.00 | 42.53 |
| ATOM | 3899 | CB  | LEU | A | 491 | 40.984 | 53.528 | 77.421 | 1.00 | 44.89 |
| ATOM | 3900 | CG  | LEU | A | 491 | 39.794 | 53.747 | 78.338 | 1.00 | 48.31 |
| ATOM | 3901 | CD1 | LEU | A | 491 | 38.558 | 54.171 | 77.552 | 1.00 | 49.16 |
| ATOM | 3902 | CD2 | LEU | A | 491 | 39.377 | 52.494 | 79.125 | 1.00 | 39.24 |
| ATOM | 3903 | N   | LYS | A | 492 | 43.958 | 52.403 | 76.754 | 1.00 | 42.32 |
| ATOM | 3904 | CA  | LYS | A | 492 | 44.999 | 52.320 | 75.696 | 1.00 | 44.57 |
| ATOM | 3905 | C   | LYS | A | 492 | 44.826 | 51.165 | 74.680 | 1.00 | 49.08 |
| ATOM | 3906 | O   | LYS | A | 492 | 44.810 | 51.343 | 73.473 | 1.00 | 49.66 |
| ATOM | 3907 | CB  | LYS | A | 492 | 46.359 | 52.    |        |      |       |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 3923 | O   | LEU | A | 494 | 39.897 | 50.029 | 72.863 | 1.00 | 38.93 |
| ATOM | 3924 | CB  | LEU | A | 494 | 40.098 | 49.125 | 75.733 | 1.00 | 32.52 |
| ATOM | 3925 | CG  | LEU | A | 494 | 40.376 | 48.433 | 77.063 | 1.00 | 30.66 |
| ATOM | 3926 | CD1 | LEU | A | 494 | 39.229 | 48.580 | 78.052 | 1.00 | 30.39 |
| ATOM | 3927 | CD2 | LEU | A | 494 | 40.611 | 46.925 | 76.918 | 1.00 | 23.54 |
| ATOM | 3928 | N   | SER | A | 495 | 39.477 | 47.825 | 72.631 | 1.00 | 25.56 |
| ATOM | 3929 | CA  | SER | A | 495 | 38.674 | 48.017 | 71.457 | 1.00 | 22.23 |
| ATOM | 3930 | C   | SER | A | 495 | 37.344 | 48.670 | 71.856 | 1.00 | 31.27 |
| ATOM | 3931 | O   | SER | A | 495 | 36.968 | 48.706 | 73.038 | 1.00 | 31.21 |
| ATOM | 3932 | CB  | SER | A | 495 | 38.380 | 46.705 | 70.795 | 1.00 | 20.88 |
| ATOM | 3933 | OG  | SER | A | 495 | 37.192 | 46.143 | 71.317 | 1.00 | 33.60 |
| ATOM | 3934 | N   | SER | A | 496 | 36.627 | 49.184 | 70.865 | 1.00 | 29.48 |
| ATOM | 3935 | CA  | SER | A | 496 | 35.363 | 49.821 | 71.139 | 1.00 | 26.67 |
| ATOM | 3936 | C   | SER | A | 496 | 34.495 | 48.747 | 71.744 | 1.00 | 29.54 |
| ATOM | 3937 | O   | SER | A | 496 | 33.744 | 48.960 | 72.697 | 1.00 | 24.80 |
| ATOM | 3938 | CB  | SER | A | 496 | 34.760 | 50.441 | 69.894 | 1.00 | 24.67 |
| ATOM | 3939 | OG  | SER | A | 496 | 33.749 | 49.597 | 69.397 | 1.00 | 48.80 |
| ATOM | 3940 | N   | HIS | A | 497 | 34.674 | 47.547 | 71.219 | 1.00 | 26.61 |
| ATOM | 3941 | CA  | HIS | A | 497 | 33.949 | 46.383 | 71.750 | 1.00 | 29.22 |
| ATOM | 3942 | C   | HIS | A | 497 | 34.156 | 46.148 | 73.275 | 1.00 | 37.24 |
| ATOM | 3943 | O   | HIS | A | 497 | 33.238 | 45.863 | 74.041 | 1.00 | 38.21 |
| ATOM | 3944 | CB  | HIS | A | 497 | 34.364 | 45.106 | 70.978 | 1.00 | 30.69 |
| ATOM | 3945 | CG  | HIS | A | 497 | 34.182 | 45.348 | 69.545 | 1.00 | 34.29 |
| ATOM | 3946 | ND1 | HIS | A | 497 | 32.943 | 45.204 | 68.962 | 1.00 | 35.42 |
| ATOM | 3947 | CD2 | HIS | A | 497 | 35.054 | 45.833 | 68.622 | 1.00 | 36.68 |
| ATOM | 3948 | CE1 | HIS | A | 497 | 33.075 | 45.531 | 67.702 | 1.00 | 35.05 |
| ATOM | 3949 | NE2 | HIS | A | 497 | 34.330 | 45.932 | 67.462 | 1.00 | 35.88 |
| ATOM | 3950 | N   | GLN | A | 498 | 35.406 | 46.243 | 73.715 | 1.00 | 33.56 |
| ATOM | 3951 | CA  | GLN | A | 498 | 35.737 | 46.008 | 75.094 | 1.00 | 29.69 |
| ATOM | 3952 | C   | GLN | A | 498 | 35.263 | 47.122 | 75.965 | 1.00 | 27.11 |
| ATOM | 3953 | O   | GLN | A | 498 | 34.842 | 46.930 | 77.089 | 1.00 | 23.92 |
| ATOM | 3954 | CB  | GLN | A | 498 | 37.221 | 45.659 | 75.248 | 1.00 | 29.95 |
| ATOM | 3955 | CG  | GLN | A | 498 | 37.582 | 44.317 | 74.544 | 1.00 | 25.78 |
| ATOM | 3956 | CD  | GLN | A | 498 | 39.074 | 44.084 | 74.535 | 1.00 | 28.64 |
| ATOM | 3957 | OE1 | GLN | A | 498 | 39.796 | 44.891 | 73.960 | 1.00 | 26.62 |
| ATOM | 3958 | NE2 | GLN | A | 498 | 39.561 | 43.049 | 75.218 | 1.00 | 20.96 |
| ATOM | 3959 | N   | LEU | A | 499 | 35.289 | 48.301 | 75.431 | 1.00 | 27.13 |
| ATOM | 3960 | CA  | LEU | A | 499 | 34.819 | 49.396 | 76.229 | 1.00 | 29.32 |
| ATOM | 3961 | C   | LEU | A | 499 | 33.351 | 49.162 | 76.632 | 1.00 | 28.39 |
| ATOM | 3962 | O   | LEU | A | 499 | 32.893 | 49.361 | 77.780 | 1.00 | 29.41 |
| ATOM | 3963 | CB  | LEU | A | 499 | 34.991 | 50.709 | 75.436 | 1.00 | 31.70 |
| ATOM | 3964 | CG  | LEU | A | 499 | 36.242 | 51.512 | 75.788 | 1.00 | 39.76 |
| ATOM | 3965 | CD1 | LEU | A | 499 | 37.335 | 50.572 | 76.278 | 1.00 | 42.91 |
| ATOM | 3966 | CD2 | LEU | A | 499 | 36.718 | 52.268 | 74.555 | 1.00 | 39.08 |
| ATOM | 3967 | N   | ASN | A | 500 | 32.606 | 48.737 | 75.642 | 1.00 | 15.23 |
| ATOM | 3968 | CA  | ASN | A | 500 | 31.213 | 48.508 | 75.828 | 1.00 | 13.44 |
| ATOM | 3969 | C   | ASN | A | 500 | 30.919 | 47.455 | 76.864 | 1.00 | 18.98 |
| ATOM | 3970 | O   | ASN | A | 500 | 29.997 | 47.602 | 77.705 | 1.00 | 19.01 |
| ATOM | 3971 | CB  | ASN | A | 500 | 30.604 | 48.129 | 74.476 | 1.00 | 12.21 |
| ATOM | 3972 | CG  | ASN | A | 500 | 29.093 | 48.214 | 74.426 | 1.00 | 37.49 |
| ATOM | 3973 | OD1 | ASN | A | 500 | 28.433 | 49.151 | 74.930 | 1.00 | 36.17 |
| ATOM | 3974 | ND2 | ASN | A | 500 | 28.542 | 47.218 | 73.787 | 1.00 | 18.34 |
| ATOM | 3975 | N   | GLU | A | 501 | 31.699 | 46.366 | 76.743 | 1.00 | 14.20 |
| ATOM | 3976 | CA  | GLU | A | 501 | 31.626 | 45.224 | 77.625 | 1.00 | 13.27 |
| ATOM | 3977 | C   | GLU | A | 501 | 31.948 | 45.676 | 79.063 | 1.00 | 21.59 |
| ATOM | 3978 | O   | GLU | A | 501 | 31.175 | 45.463 | 80.009 | 1.00 | 25.02 |
| ATOM | 3979 | CB  | GLU | A | 501 | 32.446 | 44.057 | 77.053 | 1.00 | 14.95 |
| ATOM | 3980 | CG  | GLU | A | 501 | 32.371 | 42.827 | 77.989 | 1.00 | 30.40 |



60122140-022699

|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 3981 | CD  | GLU | A | 501 | 30.946 | 42.399 | 78.199 | 1.00 | 39.28 |
| ATOM | 3982 | OE1 | GLU | A | 501 | 30.050 | 42.672 | 77.413 | 1.00 | 76.70 |
| ATOM | 3983 | OE2 | GLU | A | 501 | 30.780 | 41.694 | 79.292 | 1.00 | 46.10 |
| ATOM | 3984 | N   | PHE | A | 502 | 33.059 | 46.400 | 79.226 | 1.00 | 18.07 |
| ATOM | 3985 | CA  | PHE | A | 502 | 33.395 | 46.952 | 80.530 | 1.00 | 21.54 |
| ATOM | 3986 | C   | PHE | A | 502 | 32.179 | 47.679 | 81.125 | 1.00 | 23.38 |
| ATOM | 3987 | O   | PHE | A | 502 | 31.786 | 47.491 | 82.301 | 1.00 | 21.47 |
| ATOM | 3988 | CB  | PHE | A | 502 | 34.507 | 48.012 | 80.327 | 1.00 | 26.05 |
| ATOM | 3989 | CG  | PHE | A | 502 | 34.590 | 49.082 | 81.393 | 1.00 | 30.41 |
| ATOM | 3990 | CD1 | PHE | A | 502 | 35.085 | 48.781 | 82.662 | 1.00 | 29.68 |
| ATOM | 3991 | CD2 | PHE | A | 502 | 34.211 | 50.402 | 81.132 | 1.00 | 39.16 |
| ATOM | 3992 | CE1 | PHE | A | 502 | 35.183 | 49.773 | 83.638 | 1.00 | 31.12 |
| ATOM | 3993 | CE2 | PHE | A | 502 | 34.305 | 51.414 | 82.096 | 1.00 | 40.46 |
| ATOM | 3994 | CZ  | PHE | A | 502 | 34.812 | 51.090 | 83.352 | 1.00 | 35.41 |
| ATOM | 3995 | N   | LEU | A | 503 | 31.613 | 48.557 | 80.288 | 1.00 | 18.39 |
| ATOM | 3996 | CA  | LEU | A | 503 | 30.487 | 49.343 | 80.692 | 1.00 | 22.78 |
| ATOM | 3997 | C   | LEU | A | 503 | 29.337 | 48.491 | 81.178 | 1.00 | 31.04 |
| ATOM | 3998 | O   | LEU | A | 503 | 28.768 | 48.784 | 82.243 | 1.00 | 29.23 |
| ATOM | 3999 | CB  | LEU | A | 503 | 30.002 | 50.325 | 79.619 | 1.00 | 24.68 |
| ATOM | 4000 | CG  | LEU | A | 503 | 30.888 | 51.571 | 79.465 | 1.00 | 27.47 |
| ATOM | 4001 | CD1 | LEU | A | 503 | 30.415 | 52.376 | 78.259 | 1.00 | 24.86 |
| ATOM | 4002 | CD2 | LEU | A | 503 | 30.860 | 52.420 | 80.733 | 1.00 | 20.54 |
| ATOM | 4003 | N   | ALA | A | 504 | 29.012 | 47.444 | 80.378 | 1.00 | 27.79 |
| ATOM | 4004 | CA  | ALA | A | 504 | 27.911 | 46.474 | 80.643 | 1.00 | 24.63 |
| ATOM | 4005 | C   | ALA | A | 504 | 28.140 | 45.752 | 81.939 | 1.00 | 27.71 |
| ATOM | 4006 | O   | ALA | A | 504 | 27.265 | 45.577 | 82.817 | 1.00 | 28.62 |
| ATOM | 4007 | CB  | ALA | A | 504 | 27.762 | 45.482 | 79.496 | 1.00 | 23.87 |
| ATOM | 4008 | N   | GLN | A | 505 | 29.382 | 45.344 | 82.066 | 1.00 | 22.16 |
| ATOM | 4009 | CA  | GLN | A | 505 | 29.738 | 44.710 | 83.299 | 1.00 | 21.02 |
| ATOM | 4010 | C   | GLN | A | 505 | 29.489 | 45.737 | 84.423 | 1.00 | 31.26 |
| ATOM | 4011 | O   | GLN | A | 505 | 28.787 | 45.507 | 85.413 | 1.00 | 32.31 |
| ATOM | 4012 | CB  | GLN | A | 505 | 31.202 | 44.209 | 83.270 | 1.00 | 18.95 |
| ATOM | 4013 | CG  | GLN | A | 505 | 31.367 | 42.881 | 82.495 | 1.00 | 13.72 |
| ATOM | 4014 | CD  | GLN | A | 505 | 32.806 | 42.549 | 82.136 | 1.00 | 31.75 |
| ATOM | 4015 | OE1 | GLN | A | 505 | 33.796 | 42.969 | 82.768 | 1.00 | 43.14 |
| ATOM | 4016 | NE2 | GLN | A | 505 | 32.923 | 41.781 | 81.085 | 1.00 | 39.34 |
| ATOM | 4017 | N   | THR | A | 506 | 30.056 | 46.918 | 84.263 | 1.00 | 25.95 |
| ATOM | 4018 | CA  | THR | A | 506 | 29.855 | 47.864 | 85.302 | 1.00 | 23.64 |
| ATOM | 4019 | C   | THR | A | 506 | 28.411 | 48.101 | 85.579 | 1.00 | 23.89 |
| ATOM | 4020 | O   | THR | A | 506 | 27.923 | 47.999 | 86.696 | 1.00 | 22.75 |
| ATOM | 4021 | CB  | THR | A | 506 | 30.600 | 49.130 | 85.008 | 1.00 | 23.72 |
| ATOM | 4022 | OG1 | THR | A | 506 | 31.938 | 48.749 | 84.742 | 1.00 | 27.18 |
| ATOM | 4023 | CG2 | THR | A | 506 | 30.502 | 49.961 | 86.260 | 1.00 | 11.12 |
| ATOM | 4024 | N   | LEU | A | 507 | 27.727 | 48.408 | 84.518 | 1.00 | 17.92 |
| ATOM | 4025 | CA  | LEU | A | 507 | 26.334 | 48.683 | 84.604 | 1.00 | 17.22 |
| ATOM | 4026 | C   | LEU | A | 507 | 25.618 | 47.683 | 85.442 | 1.00 | 25.65 |
| ATOM | 4027 | O   | LEU | A | 507 | 24.816 | 48.073 | 86.266 | 1.00 | 27.85 |
| ATOM | 4028 | CB  | LEU | A | 507 | 25.693 | 48.686 | 83.224 | 1.00 | 17.85 |
| ATOM | 4029 | CG  | LEU | A | 507 | 24.207 | 48.930 | 83.336 | 1.00 | 21.02 |
| ATOM | 4030 | CD1 | LEU | A | 507 | 23.974 | 50.290 | 83.970 | 1.00 | 22.48 |
| ATOM | 4031 | CD2 | LEU | A | 507 | 23.599 | 48.919 | 81.949 | 1.00 | 15.25 |
| ATOM | 4032 | N   | GLN | A | 508 | 25.878 | 46.395 | 85.194 | 1.00 | 21.35 |
| ATOM | 4033 | CA  | GLN | A | 508 | 25.215 | 45.333 | 85.979 | 1.00 | 18.08 |
| ATOM | 4034 | C   | GLN | A | 508 | 25.386 | 45.561 | 87.508 | 1.00 | 34.24 |
| ATOM | 4035 | O   | GLN | A | 508 | 24.653 | 45.017 | 88.343 | 1.00 | 34.04 |
| ATOM | 4036 | CB  | GLN | A | 508 | 25.713 | 43.917 | 85.608 | 1.00 | 10.94 |
| ATOM | 4037 | CG  | GLN | A | 508 | 25.366 | 43.446 | 84.191 | 1.00 | 26.42 |
| ATOM | 4038 | CD  | GLN | A | 508 | 25.635 | 41.944 | 84.002 | 1.00 | 52.93 |



|      |      |     |     |   |     |        |        |        |      |        |
|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
| ATOM | 4039 | OE1 | GLN | A | 508 | 26.550 | 41.396 | 84.628 | 1.00 | 32.89  |
| ATOM | 4040 | NE2 | GLN | A | 508 | 24.864 | 41.252 | 83.147 | 1.00 | 34.36  |
| ATOM | 4041 | N   | ARG | A | 509 | 26.380 | 46.361 | 87.901 | 1.00 | 33.73  |
| ATOM | 4042 | CA  | ARG | A | 509 | 26.600 | 46.614 | 89.328 | 1.00 | 32.53  |
| ATOM | 4043 | C   | ARG | A | 509 | 26.153 | 48.016 | 89.727 | 1.00 | 33.63  |
| ATOM | 4044 | O   | ARG | A | 509 | 26.509 | 48.522 | 90.777 | 1.00 | 31.08  |
| ATOM | 4045 | CB  | ARG | A | 509 | 28.055 | 46.440 | 89.760 | 1.00 | 29.22  |
| ATOM | 4046 | CG  | ARG | A | 509 | 28.553 | 45.014 | 89.733 | 1.00 | 29.78  |
| ATOM | 4047 | CD  | ARG | A | 509 | 27.744 | 44.054 | 90.609 | 1.00 | 30.86  |
| ATOM | 4048 | NE  | ARG | A | 509 | 28.533 | 43.602 | 91.756 | 1.00 | 82.23  |
| ATOM | 4049 | CZ  | ARG | A | 509 | 29.842 | 43.274 | 91.726 | 1.00 | 100.00 |
| ATOM | 4050 | NH1 | ARG | A | 509 | 30.579 | 43.315 | 90.613 | 1.00 | 92.85  |
| ATOM | 4051 | NH2 | ARG | A | 509 | 30.430 | 42.881 | 92.855 | 1.00 | 91.85  |
| ATOM | 4052 | N   | ALA | A | 510 | 25.384 | 48.659 | 88.880 | 1.00 | 32.59  |
| ATOM | 4053 | CA  | ALA | A | 510 | 24.952 | 49.985 | 89.215 | 1.00 | 32.51  |
| ATOM | 4054 | C   | ALA | A | 510 | 24.151 | 49.845 | 90.479 | 1.00 | 34.97  |
| ATOM | 4055 | O   | ALA | A | 510 | 23.601 | 48.785 | 90.693 | 1.00 | 37.57  |
| ATOM | 4056 | CB  | ALA | A | 510 | 24.189 | 50.622 | 88.063 | 1.00 | 32.91  |
| ATOM | 4057 | N   | PRO | A | 511 | 24.174 | 50.856 | 91.334 | 1.00 | 25.14  |
| ATOM | 4058 | CA  | PRO | A | 511 | 24.867 | 52.102 | 91.052 | 1.00 | 21.00  |
| ATOM | 4059 | C   | PRO | A | 511 | 26.217 | 52.178 | 91.694 | 1.00 | 29.23  |
| ATOM | 4060 | O   | PRO | A | 511 | 26.445 | 51.601 | 92.723 | 1.00 | 28.16  |
| ATOM | 4061 | CB  | PRO | A | 511 | 24.102 | 53.169 | 91.818 | 1.00 | 21.55  |
| ATOM | 4062 | CG  | PRO | A | 511 | 23.316 | 52.432 | 92.886 | 1.00 | 28.68  |
| ATOM | 4063 | CD  | PRO | A | 511 | 23.169 | 50.995 | 92.407 | 1.00 | 25.16  |
| ATOM | 4064 | N   | LEU | A | 512 | 27.094 | 52.968 | 91.109 | 1.00 | 32.95  |
| ATOM | 4065 | CA  | LEU | A | 512 | 28.394 | 53.188 | 91.686 | 1.00 | 33.42  |
| ATOM | 4066 | C   | LEU | A | 512 | 28.287 | 54.512 | 92.397 | 1.00 | 38.65  |
| ATOM | 4067 | O   | LEU | A | 512 | 27.388 | 55.305 | 92.114 | 1.00 | 40.69  |
| ATOM | 4068 | CB  | LEU | A | 512 | 29.453 | 53.350 | 90.587 | 1.00 | 34.40  |
| ATOM | 4069 | CG  | LEU | A | 512 | 30.178 | 52.049 | 90.216 | 1.00 | 40.13  |
| ATOM | 4070 | CD1 | LEU | A | 512 | 29.222 | 51.086 | 89.508 | 1.00 | 39.04  |
| ATOM | 4071 | CD2 | LEU | A | 512 | 31.322 | 52.385 | 89.273 | 1.00 | 44.61  |
| ATOM | 4072 | N   | PRO | A | 513 | 29.196 | 54.781 | 93.312 | 1.00 | 31.05  |
| ATOM | 4073 | CA  | PRO | A | 513 | 29.167 | 56.058 | 94.008 | 1.00 | 27.16  |
| ATOM | 4074 | C   | PRO | A | 513 | 29.296 | 57.203 | 93.019 | 1.00 | 23.76  |
| ATOM | 4075 | O   | PRO | A | 513 | 30.121 | 57.182 | 92.118 | 1.00 | 27.17  |
| ATOM | 4076 | CB  | PRO | A | 513 | 30.387 | 56.013 | 94.948 | 1.00 | 25.59  |
| ATOM | 4077 | CG  | PRO | A | 513 | 30.702 | 54.542 | 95.149 | 1.00 | 27.14  |
| ATOM | 4078 | CD  | PRO | A | 513 | 30.030 | 53.779 | 94.032 | 1.00 | 25.00  |
| ATOM | 4079 | N   | LEU | A | 514 | 28.478 | 58.203 | 93.185 | 1.00 | 22.92  |
| ATOM | 4080 | CA  | LEU | A | 514 | 28.516 | 59.350 | 92.279 | 1.00 | 27.55  |
| ATOM | 4081 | C   | LEU | A | 514 | 29.930 | 59.766 | 91.940 | 1.00 | 31.95  |
| ATOM | 4082 | O   | LEU | A | 514 | 30.287 | 59.908 | 90.765 | 1.00 | 37.11  |
| ATOM | 4083 | CB  | LEU | A | 514 | 27.673 | 60.564 | 92.741 | 1.00 | 30.03  |
| ATOM | 4084 | CG  | LEU | A | 514 | 27.428 | 61.626 | 91.648 | 1.00 | 32.87  |
| ATOM | 4085 | CD1 | LEU | A | 514 | 26.648 | 61.082 | 90.440 | 1.00 | 28.48  |
| ATOM | 4086 | CD2 | LEU | A | 514 | 26.699 | 62.780 | 92.272 | 1.00 | 31.16  |
| ATOM | 4087 | N   | GLY | A | 515 | 30.731 | 59.989 | 92.979 | 1.00 | 24.42  |
| ATOM | 4088 | CA  | GLY | A | 515 | 32.131 | 60.384 | 92.811 | 1.00 | 25.59  |
| ATOM | 4089 | C   | GLY | A | 515 | 32.902 | 59.472 | 91.835 | 1.00 | 33.83  |
| ATOM | 4090 | O   | GLY | A | 515 | 33.746 | 59.914 | 91.035 | 1.00 | 35.67  |
| ATOM | 4091 | N   | HIS | A | 516 | 32.602 | 58.180 | 91.891 | 1.00 | 26.40  |
| ATOM | 4092 | CA  | HIS | A | 516 | 33.257 | 57.255 | 90.998 | 1.00 | 25.86  |
| ATOM | 4093 | C   | HIS | A | 516 | 32.911 | 57.578 | 89.560 | 1.00 | 27.62  |
| ATOM | 4094 | O   | HIS | A | 516 | 33.786 | 57.596 | 88.695 | 1.00 | 28.67  |
| ATOM | 4095 | CB  | HIS | A | 516 | 32.826 | 55.814 | 91.282 | 1.00 | 25.39  |
| ATOM | 4096 | CG  | HIS | A | 516 | 33.452 | 55.283 | 92.505 | 1.00 | 27.96  |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 4097 | ND1 | HIS | A | 516 | 33.635 | 56.092 | 93.602 | 1.00 | 30.14 |
| ATOM | 4098 | CD2 | HIS | A | 516 | 33.929 | 54.037 | 92.791 | 1.00 | 27.79 |
| ATOM | 4099 | CE1 | HIS | A | 516 | 34.205 | 55.336 | 94.534 | 1.00 | 27.58 |
| ATOM | 4100 | NE2 | HIS | A | 516 | 34.390 | 54.099 | 94.085 | 1.00 | 27.02 |
| ATOM | 4101 | N   | ILE | A | 517 | 31.617 | 57.815 | 89.315 | 1.00 | 21.40 |
| ATOM | 4102 | CA  | ILE | A | 517 | 31.137 | 58.107 | 87.973 | 1.00 | 22.75 |
| ATOM | 4103 | C   | ILE | A | 517 | 31.706 | 59.424 | 87.462 | 1.00 | 31.09 |
| ATOM | 4104 | O   | ILE | A | 517 | 32.246 | 59.558 | 86.352 | 1.00 | 28.78 |
| ATOM | 4105 | CB  | ILE | A | 517 | 29.601 | 58.024 | 87.930 | 1.00 | 27.12 |
| ATOM | 4106 | CG1 | ILE | A | 517 | 29.225 | 56.610 | 88.312 | 1.00 | 29.40 |
| ATOM | 4107 | CG2 | ILE | A | 517 | 29.013 | 58.285 | 86.536 | 1.00 | 25.49 |
| ATOM | 4108 | CD1 | ILE | A | 517 | 29.305 | 55.665 | 87.105 | 1.00 | 34.77 |
| ATOM | 4109 | N   | LYS | A | 518 | 31.589 | 60.416 | 88.308 | 1.00 | 27.28 |
| ATOM | 4110 | CA  | LYS | A | 518 | 32.108 | 61.690 | 87.955 | 1.00 | 23.77 |
| ATOM | 4111 | C   | LYS | A | 518 | 33.558 | 61.482 | 87.485 | 1.00 | 24.03 |
| ATOM | 4112 | O   | LYS | A | 518 | 33.982 | 61.831 | 86.391 | 1.00 | 26.08 |
| ATOM | 4113 | CB  | LYS | A | 518 | 32.038 | 62.557 | 89.210 | 1.00 | 24.00 |
| ATOM | 4114 | CG  | LYS | A | 518 | 30.641 | 63.060 | 89.591 | 1.00 | 19.24 |
| ATOM | 4115 | CD  | LYS | A | 518 | 30.721 | 64.276 | 90.537 | 1.00 | 27.93 |
| ATOM | 4116 | CE  | LYS | A | 518 | 29.379 | 64.877 | 90.962 | 1.00 | 37.11 |
| ATOM | 4117 | NZ  | LYS | A | 518 | 28.924 | 65.988 | 90.104 | 1.00 | 52.30 |
| ATOM | 4118 | N   | ARG | A | 519 | 34.322 | 60.899 | 88.361 | 1.00 | 17.90 |
| ATOM | 4119 | CA  | ARG | A | 519 | 35.703 | 60.636 | 88.098 | 1.00 | 20.80 |
| ATOM | 4120 | C   | ARG | A | 519 | 35.862 | 59.874 | 86.802 | 1.00 | 28.98 |
| ATOM | 4121 | O   | ARG | A | 519 | 36.812 | 60.084 | 86.051 | 1.00 | 29.86 |
| ATOM | 4122 | CB  | ARG | A | 519 | 36.313 | 59.844 | 89.276 | 1.00 | 20.56 |
| ATOM | 4123 | CG  | ARG | A | 519 | 37.721 | 59.308 | 89.036 | 1.00 | 29.02 |
| ATOM | 4124 | CD  | ARG | A | 519 | 38.668 | 60.320 | 88.404 | 1.00 | 41.17 |
| ATOM | 4125 | NE  | ARG | A | 519 | 40.086 | 60.008 | 88.616 | 1.00 | 59.84 |
| ATOM | 4126 | CZ  | ARG | A | 519 | 41.076 | 60.858 | 88.349 | 1.00 | 50.77 |
| ATOM | 4127 | NH1 | ARG | A | 519 | 40.838 | 62.073 | 87.880 | 1.00 | 31.21 |
| ATOM | 4128 | NH2 | ARG | A | 519 | 42.329 | 60.486 | 88.543 | 1.00 | 31.86 |
| ATOM | 4129 | N   | MET | A | 520 | 34.937 | 58.956 | 86.565 | 1.00 | 25.08 |
| ATOM | 4130 | CA  | MET | A | 520 | 34.979 | 58.121 | 85.379 | 1.00 | 24.56 |
| ATOM | 4131 | C   | MET | A | 520 | 34.906 | 58.918 | 84.086 | 1.00 | 29.37 |
| ATOM | 4132 | O   | MET | A | 520 | 35.651 | 58.687 | 83.114 | 1.00 | 27.92 |
| ATOM | 4133 | CB  | MET | A | 520 | 33.905 | 57.007 | 85.442 | 1.00 | 26.98 |
| ATOM | 4134 | CG  | MET | A | 520 | 34.082 | 55.902 | 84.399 | 1.00 | 28.02 |
| ATOM | 4135 | SD  | MET | A | 520 | 32.830 | 54.591 | 84.479 | 1.00 | 27.87 |
| ATOM | 4136 | CE  | MET | A | 520 | 33.246 | 53.825 | 86.070 | 1.00 | 22.09 |
| ATOM | 4137 | N   | GLN | A | 521 | 33.982 | 59.864 | 84.067 | 1.00 | 28.32 |
| ATOM | 4138 | CA  | GLN | A | 521 | 33.838 | 60.672 | 82.886 | 1.00 | 28.34 |
| ATOM | 4139 | C   | GLN | A | 521 | 35.067 |        |        |      |       |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 4155 | N   | VAL | A | 523 | 38.188 | 60.739 | 83.552 | 1.00 | 40.13 |
| ATOM | 4156 | CA  | VAL | A | 523 | 39.401 | 60.136 | 83.058 | 1.00 | 37.49 |
| ATOM | 4157 | C   | VAL | A | 523 | 39.205 | 59.351 | 81.778 | 1.00 | 38.88 |
| ATOM | 4158 | O   | VAL | A | 523 | 40.195 | 59.016 | 81.138 | 1.00 | 40.21 |
| ATOM | 4159 | CB  | VAL | A | 523 | 40.184 | 59.370 | 84.102 | 1.00 | 40.01 |
| ATOM | 4160 | CG1 | VAL | A | 523 | 40.231 | 60.165 | 85.413 | 1.00 | 39.12 |
| ATOM | 4161 | CG2 | VAL | A | 523 | 39.534 | 58.017 | 84.320 | 1.00 | 39.82 |
| ATOM | 4162 | N   | TYR | A | 524 | 37.952 | 59.048 | 81.379 | 1.00 | 30.35 |
| ATOM | 4163 | CA  | TYR | A | 524 | 37.801 | 58.330 | 80.114 | 1.00 | 28.11 |
| ATOM | 4164 | C   | TYR | A | 524 | 37.061 | 59.144 | 79.074 | 1.00 | 33.14 |
| ATOM | 4165 | O   | TYR | A | 524 | 37.076 | 58.802 | 77.908 | 1.00 | 35.84 |
| ATOM | 4166 | CB  | TYR | A | 524 | 37.281 | 56.878 | 80.119 | 1.00 | 25.56 |
| ATOM | 4167 | CG  | TYR | A | 524 | 37.941 | 55.960 | 81.111 | 1.00 | 20.87 |
| ATOM | 4168 | CD1 | TYR | A | 524 | 39.324 | 55.938 | 81.258 | 1.00 | 21.59 |
| ATOM | 4169 | CD2 | TYR | A | 524 | 37.170 | 55.083 | 81.879 | 1.00 | 19.80 |
| ATOM | 4170 | CE1 | TYR | A | 524 | 39.905 | 55.063 | 82.176 | 1.00 | 25.64 |
| ATOM | 4171 | CE2 | TYR | A | 524 | 37.731 | 54.227 | 82.827 | 1.00 | 18.61 |
| ATOM | 4172 | CZ  | TYR | A | 524 | 39.116 | 54.231 | 82.969 | 1.00 | 19.81 |
| ATOM | 4173 | OH  | TYR | A | 524 | 39.706 | 53.402 | 83.863 | 1.00 | 23.92 |
| ATOM | 4174 | N   | ASN | A | 525 | 36.416 | 60.221 | 79.496 | 1.00 | 25.98 |
| ATOM | 4175 | CA  | ASN | A | 525 | 35.687 | 61.088 | 78.588 | 1.00 | 25.01 |
| ATOM | 4176 | C   | ASN | A | 525 | 34.661 | 60.354 | 77.735 | 1.00 | 29.86 |
| ATOM | 4177 | O   | ASN | A | 525 | 34.533 | 60.535 | 76.499 | 1.00 | 29.39 |
| ATOM | 4178 | CB  | ASN | A | 525 | 36.637 | 61.922 | 77.739 | 1.00 | 29.55 |
| ATOM | 4179 | CG  | ASN | A | 525 | 35.949 | 62.980 | 76.894 | 1.00 | 30.32 |
| ATOM | 4180 | OD1 | ASN | A | 525 | 36.460 | 63.332 | 75.850 | 1.00 | 32.77 |
| ATOM | 4181 | ND2 | ASN | A | 525 | 34.822 | 63.527 | 77.344 | 1.00 | 13.80 |
| ATOM | 4182 | N   | PHE | A | 526 | 33.924 | 59.512 | 78.436 | 1.00 | 24.21 |
| ATOM | 4183 | CA  | PHE | A | 526 | 32.900 | 58.745 | 77.807 | 1.00 | 25.14 |
| ATOM | 4184 | C   | PHE | A | 526 | 31.846 | 59.631 | 77.214 | 1.00 | 31.74 |
| ATOM | 4185 | O   | PHE | A | 526 | 31.161 | 59.241 | 76.272 | 1.00 | 34.99 |
| ATOM | 4186 | CB  | PHE | A | 526 | 32.256 | 57.732 | 78.781 | 1.00 | 26.60 |
| ATOM | 4187 | CG  | PHE | A | 526 | 33.115 | 56.499 | 78.978 | 1.00 | 23.82 |
| ATOM | 4188 | CD1 | PHE | A | 526 | 34.017 | 56.080 | 78.000 | 1.00 | 25.00 |
| ATOM | 4189 | CD2 | PHE | A | 526 | 33.031 | 55.767 | 80.159 | 1.00 | 21.74 |
| ATOM | 4190 | CE1 | PHE | A | 526 | 34.783 | 54.927 | 78.173 | 1.00 | 27.63 |
| ATOM | 4191 | CE2 | PHE | A | 526 | 33.817 | 54.634 | 80.370 | 1.00 | 25.42 |
| ATOM | 4192 | CZ  | PHE | A | 526 | 34.683 | 54.202 | 79.364 | 1.00 | 25.28 |
| ATOM | 4193 | N   | ASN | A | 527 | 31.689 | 60.815 | 77.760 | 1.00 | 28.22 |
| ATOM | 4194 | CA  | ASN | A | 527 | 30.657 | 61.688 | 77.214 | 1.00 | 31.18 |
| ATOM | 4195 | C   | ASN | A | 527 | 30.884 | 62.046 | 75.744 | 1.00 | 33.17 |
| ATOM | 4196 | O   | ASN | A | 527 | 29.965 | 62.394 | 74.999 | 1.00 | 30.80 |
| ATOM | 4197 | CB  | ASN | A | 527 | 30.479 | 62.967 | 78.052 | 1.00 | 36.41 |
| ATOM | 4198 | CG  | ASN | A | 527 | 29.638 | 62.752 | 79.292 | 1.00 | 46.99 |
| ATOM | 4199 | OD1 | ASN | A | 527 | 29.647 | 63.571 | 80.209 | 1.00 | 36.82 |
| ATOM | 4200 | ND2 | ASN | A | 527 | 28.922 | 61.636 | 79.338 | 1.00 | 43.55 |
| ATOM | 4201 | N   | ALA | A | 528 | 32.136 | 61.947 | 75.348 | 1.00 | 27.46 |
| ATOM | 4202 | CA  | ALA | A | 528 | 32.581 | 62.278 | 74.005 | 1.00 | 26.48 |
| ATOM | 4203 | C   | ALA | A | 528 | 32.335 | 61.188 | 72.950 | 1.00 | 32.09 |
| ATOM | 4204 | O   | ALA | A | 528 | 32.420 | 61.404 | 71.753 | 1.00 | 32.09 |
| ATOM | 4205 | CB  | ALA | A | 528 | 34.076 | 62.584 | 74.105 | 1.00 | 26.04 |
| ATOM | 4206 | N   | ILE | A | 529 | 32.067 | 59.983 | 73.402 | 1.00 | 31.35 |
| ATOM | 4207 | CA  | ILE | A | 529 | 31.854 | 58.859 | 72.529 | 1.00 | 28.47 |
| ATOM | 4208 | C   | ILE | A | 529 | 30.492 | 58.904 | 71.887 | 1.00 | 35.96 |
| ATOM | 4209 | O   | ILE | A | 529 | 29.486 | 59.023 | 72.578 | 1.00 | 38.79 |
| ATOM | 4210 | CB  | ILE | A | 529 | 32.103 | 57.544 | 73.264 | 1.00 | 30.17 |
| ATOM | 4211 | CG1 | ILE | A | 529 | 33.622 | 57.291 | 73.392 | 1.00 | 31.37 |
| ATOM | 4212 | CG2 | ILE | A | 529 | 31.428 | 56.411 | 72.489 | 1.00 | 27.63 |



|      |      |     |     |   |     |        |        |        |      |        |
|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
| ATOM | 4213 | CD1 | ILE | A | 529 | 34.059 | 56.515 | 74.635 | 1.00 | 33.41  |
| ATOM | 4214 | N   | ASN | A | 530 | 30.462 | 58.806 | 70.559 | 1.00 | 34.86  |
| ATOM | 4215 | CA  | ASN | A | 530 | 29.196 | 58.841 | 69.852 | 1.00 | 36.44  |
| ATOM | 4216 | C   | ASN | A | 530 | 28.596 | 57.495 | 69.473 | 1.00 | 39.90  |
| ATOM | 4217 | O   | ASN | A | 530 | 27.452 | 57.437 | 69.043 | 1.00 | 41.37  |
| ATOM | 4218 | CB  | ASN | A | 530 | 28.951 | 60.044 | 68.928 | 1.00 | 51.44  |
| ATOM | 4219 | CG  | ASN | A | 530 | 28.461 | 61.253 | 69.732 | 1.00 | 100.00 |
| ATOM | 4220 | OD1 | ASN | A | 530 | 27.652 | 61.109 | 70.665 | 1.00 | 100.00 |
| ATOM | 4221 | ND2 | ASN | A | 530 | 28.955 | 62.442 | 69.392 | 1.00 | 91.39  |
| ATOM | 4222 | N   | ASN | A | 531 | 29.368 | 56.403 | 69.688 | 1.00 | 30.33  |
| ATOM | 4223 | CA  | ASN | A | 531 | 28.912 | 55.030 | 69.446 | 1.00 | 28.14  |
| ATOM | 4224 | C   | ASN | A | 531 | 27.696 | 54.753 | 70.360 | 1.00 | 32.80  |
| ATOM | 4225 | O   | ASN | A | 531 | 27.746 | 54.887 | 71.611 | 1.00 | 36.74  |
| ATOM | 4226 | CB  | ASN | A | 531 | 30.092 | 54.066 | 69.690 | 1.00 | 24.31  |
| ATOM | 4227 | CG  | ASN | A | 531 | 29.770 | 52.601 | 69.730 | 1.00 | 34.44  |
| ATOM | 4228 | OD1 | ASN | A | 531 | 28.795 | 52.182 | 70.359 | 1.00 | 36.49  |
| ATOM | 4229 | ND2 | ASN | A | 531 | 30.643 | 51.810 | 69.099 | 1.00 | 30.57  |
| ATOM | 4230 | N   | SER | A | 532 | 26.570 | 54.403 | 69.734 | 1.00 | 22.02  |
| ATOM | 4231 | CA  | SER | A | 532 | 25.325 | 54.183 | 70.459 | 1.00 | 19.67  |
| ATOM | 4232 | C   | SER | A | 532 | 25.323 | 53.208 | 71.627 | 1.00 | 26.15  |
| ATOM | 4233 | O   | SER | A | 532 | 24.767 | 53.475 | 72.680 | 1.00 | 26.64  |
| ATOM | 4234 | CB  | SER | A | 532 | 24.090 | 54.034 | 69.582 | 1.00 | 26.92  |
| ATOM | 4235 | OG  | SER | A | 532 | 24.294 | 53.211 | 68.452 | 1.00 | 23.59  |
| ATOM | 4236 | N   | GLU | A | 533 | 25.929 | 52.062 | 71.423 | 1.00 | 22.68  |
| ATOM | 4237 | CA  | GLU | A | 533 | 25.995 | 51.036 | 72.420 | 1.00 | 22.97  |
| ATOM | 4238 | C   | GLU | A | 533 | 26.677 | 51.569 | 73.635 | 1.00 | 30.48  |
| ATOM | 4239 | O   | GLU | A | 533 | 26.125 | 51.539 | 74.749 | 1.00 | 31.13  |
| ATOM | 4240 | CB  | GLU | A | 533 | 26.683 | 49.779 | 71.850 | 1.00 | 23.96  |
| ATOM | 4241 | CG  | GLU | A | 533 | 25.827 | 49.146 | 70.733 | 1.00 | 20.82  |
| ATOM | 4242 | CD  | GLU | A | 533 | 24.611 | 48.450 | 71.276 | 1.00 | 40.65  |
| ATOM | 4243 | OE1 | GLU | A | 533 | 24.432 | 48.256 | 72.476 | 1.00 | 36.25  |
| ATOM | 4244 | OE2 | GLU | A | 533 | 23.782 | 48.038 | 70.339 | 1.00 | 25.87  |
| ATOM | 4245 | N   | ILE | A | 534 | 27.872 | 52.101 | 73.392 | 1.00 | 26.20  |
| ATOM | 4246 | CA  | ILE | A | 534 | 28.622 | 52.672 | 74.484 | 1.00 | 26.32  |
| ATOM | 4247 | C   | ILE | A | 534 | 27.900 | 53.849 | 75.121 | 1.00 | 27.83  |
| ATOM | 4248 | O   | ILE | A | 534 | 27.697 | 53.911 | 76.326 | 1.00 | 26.54  |
| ATOM | 4249 | CB  | ILE | A | 534 | 30.051 | 53.022 | 74.102 | 1.00 | 29.16  |
| ATOM | 4250 | CG1 | ILE | A | 534 | 30.738 | 51.808 | 73.479 | 1.00 | 29.47  |
| ATOM | 4251 | CG2 | ILE | A | 534 | 30.801 | 53.458 | 75.353 | 1.00 | 28.28  |
| ATOM | 4252 | CD1 | ILE | A | 534 | 32.038 | 52.184 | 72.765 | 1.00 | 34.99  |
| ATOM | 4253 | N   | ARG | A | 535 | 27.480 | 54.805 | 74.320 | 1.00 | 24.30  |
| ATOM | 4254 | CA  | ARG | A | 535 | 26.804 | 55.898 | 74.949 | 1.00 | 22.51  |
| ATOM | 4255 | C   | ARG | A | 535 | 25.573 | 55.    |        |      |        |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 4271 | CD2 | PHE | A | 536 | 22.145 | 50.783 | 75.882 | 1.00 | 23.25 |
| ATOM | 4272 | CE1 | PHE | A | 536 | 19.926 | 52.181 | 76.847 | 1.00 | 21.23 |
| ATOM | 4273 | CE2 | PHE | A | 536 | 21.147 | 50.101 | 76.576 | 1.00 | 24.70 |
| ATOM | 4274 | CZ  | PHE | A | 536 | 20.047 | 50.811 | 77.065 | 1.00 | 20.57 |
| ATOM | 4275 | N   | ARG | A | 537 | 24.863 | 52.560 | 77.364 | 1.00 | 18.22 |
| ATOM | 4276 | CA  | ARG | A | 537 | 25.239 | 51.995 | 78.665 | 1.00 | 19.20 |
| ATOM | 4277 | C   | ARG | A | 537 | 25.932 | 52.963 | 79.618 | 1.00 | 27.62 |
| ATOM | 4278 | O   | ARG | A | 537 | 25.803 | 52.845 | 80.837 | 1.00 | 26.73 |
| ATOM | 4279 | CB  | ARG | A | 537 | 26.035 | 50.709 | 78.556 | 1.00 | 18.91 |
| ATOM | 4280 | CG  | ARG | A | 537 | 25.318 | 49.656 | 77.708 | 1.00 | 16.55 |
| ATOM | 4281 | CD  | ARG | A | 537 | 26.181 | 48.426 | 77.387 | 1.00 | 21.58 |
| ATOM | 4282 | NE  | ARG | A | 537 | 25.341 | 47.357 | 76.886 | 1.00 | 28.42 |
| ATOM | 4283 | CZ  | ARG | A | 537 | 25.060 | 47.206 | 75.609 | 1.00 | 18.29 |
| ATOM | 4284 | NH1 | ARG | A | 537 | 25.569 | 48.004 | 74.703 | 1.00 | 22.46 |
| ATOM | 4285 | NH2 | ARG | A | 537 | 24.240 | 46.236 | 75.224 | 1.00 | 25.22 |
| ATOM | 4286 | N   | TRP | A | 538 | 26.668 | 53.930 | 79.064 | 1.00 | 24.21 |
| ATOM | 4287 | CA  | TRP | A | 538 | 27.337 | 54.918 | 79.867 | 1.00 | 22.11 |
| ATOM | 4288 | C   | TRP | A | 538 | 26.274 | 55.719 | 80.550 | 1.00 | 28.09 |
| ATOM | 4289 | O   | TRP | A | 538 | 26.320 | 55.951 | 81.741 | 1.00 | 27.39 |
| ATOM | 4290 | CB  | TRP | A | 538 | 28.064 | 55.888 | 78.949 | 1.00 | 20.48 |
| ATOM | 4291 | CG  | TRP | A | 538 | 28.606 | 57.157 | 79.580 | 1.00 | 21.29 |
| ATOM | 4292 | CD1 | TRP | A | 538 | 28.641 | 58.345 | 78.968 | 1.00 | 22.86 |
| ATOM | 4293 | CD2 | TRP | A | 538 | 29.286 | 57.352 | 80.845 | 1.00 | 21.79 |
| ATOM | 4294 | NE1 | TRP | A | 538 | 29.228 | 59.270 | 79.769 | 1.00 | 22.70 |
| ATOM | 4295 | CE2 | TRP | A | 538 | 29.643 | 58.696 | 80.911 | 1.00 | 24.79 |
| ATOM | 4296 | CE3 | TRP | A | 538 | 29.574 | 56.535 | 81.946 | 1.00 | 23.35 |
| ATOM | 4297 | CZ2 | TRP | A | 538 | 30.280 | 59.248 | 82.025 | 1.00 | 25.89 |
| ATOM | 4298 | CZ3 | TRP | A | 538 | 30.203 | 57.056 | 83.046 | 1.00 | 23.35 |
| ATOM | 4299 | CH2 | TRP | A | 538 | 30.562 | 58.405 | 83.081 | 1.00 | 24.89 |
| ATOM | 4300 | N   | LEU | A | 539 | 25.303 | 56.161 | 79.758 | 1.00 | 27.31 |
| ATOM | 4301 | CA  | LEU | A | 539 | 24.229 | 56.974 | 80.306 | 1.00 | 27.18 |
| ATOM | 4302 | C   | LEU | A | 539 | 23.369 | 56.245 | 81.332 | 1.00 | 28.25 |
| ATOM | 4303 | O   | LEU | A | 539 | 22.857 | 56.822 | 82.266 | 1.00 | 27.19 |
| ATOM | 4304 | CB  | LEU | A | 539 | 23.428 | 57.812 | 79.262 | 1.00 | 26.37 |
| ATOM | 4305 | CG  | LEU | A | 539 | 24.269 | 58.682 | 78.279 | 1.00 | 25.71 |
| ATOM | 4306 | CD1 | LEU | A | 539 | 23.369 | 59.424 | 77.290 | 1.00 | 21.79 |
| ATOM | 4307 | CD2 | LEU | A | 539 | 25.146 | 59.680 | 79.011 | 1.00 | 23.51 |
| ATOM | 4308 | N   | ARG | A | 540 | 23.199 | 54.960 | 81.188 | 1.00 | 27.56 |
| ATOM | 4309 | CA  | ARG | A | 540 | 22.390 | 54.283 | 82.170 | 1.00 | 26.88 |
| ATOM | 4310 | C   | ARG | A | 540 | 23.145 | 54.229 | 83.453 | 1.00 | 31.82 |
| ATOM | 4311 | O   | ARG | A | 540 | 22.618 | 54.448 | 84.539 | 1.00 | 32.72 |
| ATOM | 4312 | CB  | ARG | A | 540 | 22.034 | 52.888 | 81.732 | 1.00 | 24.48 |
| ATOM | 4313 | CG  | ARG | A | 5   |        |        |        |      |       |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 4329 | C   | CYS | A | 542 | 23.808 | 57.996 | 85.805 | 1.00 | 32.71 |
| ATOM | 4330 | O   | CYS | A | 542 | 23.801 | 58.536 | 86.914 | 1.00 | 33.97 |
| ATOM | 4331 | CB  | CYS | A | 542 | 25.461 | 58.744 | 84.073 | 1.00 | 31.30 |
| ATOM | 4332 | SG  | CYS | A | 542 | 27.085 | 58.488 | 83.347 | 1.00 | 34.39 |
| ATOM | 4333 | N   | ILE | A | 543 | 22.711 | 57.708 | 85.125 | 1.00 | 25.61 |
| ATOM | 4334 | CA  | ILE | A | 543 | 21.382 | 57.982 | 85.643 | 1.00 | 23.12 |
| ATOM | 4335 | C   | ILE | A | 543 | 21.199 | 57.161 | 86.885 | 1.00 | 30.15 |
| ATOM | 4336 | O   | ILE | A | 543 | 20.900 | 57.645 | 87.972 | 1.00 | 30.73 |
| ATOM | 4337 | CB  | ILE | A | 543 | 20.340 | 57.627 | 84.585 | 1.00 | 23.75 |
| ATOM | 4338 | CG1 | ILE | A | 543 | 20.369 | 58.664 | 83.468 | 1.00 | 24.09 |
| ATOM | 4339 | CG2 | ILE | A | 543 | 18.955 | 57.572 | 85.182 | 1.00 | 22.99 |
| ATOM | 4340 | CD1 | ILE | A | 543 | 20.386 | 60.109 | 83.982 | 1.00 | 27.34 |
| ATOM | 4341 | N   | GLN | A | 544 | 21.440 | 55.884 | 86.695 | 1.00 | 27.99 |
| ATOM | 4342 | CA  | GLN | A | 544 | 21.320 | 54.929 | 87.756 | 1.00 | 25.72 |
| ATOM | 4343 | C   | GLN | A | 544 | 22.243 | 55.269 | 88.901 | 1.00 | 26.34 |
| ATOM | 4344 | O   | GLN | A | 544 | 22.029 | 54.826 | 90.014 | 1.00 | 26.24 |
| ATOM | 4345 | CB  | GLN | A | 544 | 21.562 | 53.512 | 87.210 | 1.00 | 26.76 |
| ATOM | 4346 | CG  | GLN | A | 544 | 20.355 | 52.955 | 86.432 | 1.00 | 17.74 |
| ATOM | 4347 | CD  | GLN | A | 544 | 20.598 | 51.604 | 85.743 | 1.00 | 32.62 |
| ATOM | 4348 | OE1 | GLN | A | 544 | 20.326 | 51.432 | 84.551 | 1.00 | 38.66 |
| ATOM | 4349 | NE2 | GLN | A | 544 | 21.063 | 50.627 | 86.494 | 1.00 | 14.93 |
| ATOM | 4350 | N   | SER | A | 545 | 23.286 | 56.033 | 88.625 | 1.00 | 21.73 |
| ATOM | 4351 | CA  | SER | A | 545 | 24.187 | 56.392 | 89.685 | 1.00 | 22.42 |
| ATOM | 4352 | C   | SER | A | 545 | 23.819 | 57.726 | 90.287 | 1.00 | 33.67 |
| ATOM | 4353 | O   | SER | A | 545 | 24.567 | 58.257 | 91.133 | 1.00 | 37.22 |
| ATOM | 4354 | CB  | SER | A | 545 | 25.646 | 56.322 | 89.338 | 1.00 | 21.57 |
| ATOM | 4355 | OG  | SER | A | 545 | 25.980 | 54.968 | 89.163 | 1.00 | 31.72 |
| ATOM | 4356 | N   | LYS | A | 546 | 22.662 | 58.251 | 89.841 | 1.00 | 23.09 |
| ATOM | 4357 | CA  | LYS | A | 546 | 22.135 | 59.490 | 90.356 | 1.00 | 20.79 |
| ATOM | 4358 | C   | LYS | A | 546 | 22.887 | 60.738 | 89.961 | 1.00 | 27.55 |
| ATOM | 4359 | O   | LYS | A | 546 | 23.001 | 61.655 | 90.771 | 1.00 | 27.95 |
| ATOM | 4360 | CB  | LYS | A | 546 | 22.126 | 59.449 | 91.881 | 1.00 | 21.71 |
| ATOM | 4361 | CG  | LYS | A | 546 | 21.498 | 58.195 | 92.484 | 1.00 | 15.90 |
| ATOM | 4362 | CD  | LYS | A | 546 | 20.245 | 57.814 | 91.731 | 1.00 | 39.84 |
| ATOM | 4363 | CE  | LYS | A | 546 | 19.355 | 56.850 | 92.498 | 1.00 | 45.16 |
| ATOM | 4364 | NZ  | LYS | A | 546 | 18.197 | 56.399 | 91.704 | 1.00 | 40.14 |
| ATOM | 4365 | N   | TRP | A | 547 | 23.414 | 60.776 | 88.753 | 1.00 | 23.26 |
| ATOM | 4366 | CA  | TRP | A | 547 | 24.141 | 61.931 | 88.289 | 1.00 | 21.90 |
| ATOM | 4367 | C   | TRP | A | 547 | 23.221 | 62.901 | 87.570 | 1.00 | 29.82 |
| ATOM | 4368 | O   | TRP | A | 547 | 22.808 | 62.679 | 86.432 | 1.00 | 34.91 |
| ATOM | 4369 | CB  | TRP | A | 547 | 25.262 | 61.500 | 87.361 | 1.00 | 21.04 |
| ATOM | 4370 | CG  | TRP | A | 547 | 26.254 | 62.591 | 87.206 | 1.00 | 22.57 |
| ATOM | 4371 | CD1 | TRP | A | 547 | 26.2   |        |        |      |       |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 4387 | OE2 | GLU | A | 548 | 19.888 | 66.450 | 91.925 | 1.00 | 57.05 |
| ATOM | 4388 | N   | ASP | A | 549 | 23.728 | 65.661 | 86.201 | 1.00 | 24.72 |
| ATOM | 4389 | CA  | ASP | A | 549 | 24.276 | 66.190 | 84.981 | 1.00 | 21.48 |
| ATOM | 4390 | C   | ASP | A | 549 | 23.914 | 65.359 | 83.795 | 1.00 | 30.08 |
| ATOM | 4391 | O   | ASP | A | 549 | 23.760 | 65.869 | 82.697 | 1.00 | 32.05 |
| ATOM | 4392 | CB  | ASP | A | 549 | 25.775 | 66.480 | 85.048 | 1.00 | 21.28 |
| ATOM | 4393 | CG  | ASP | A | 549 | 26.076 | 67.463 | 86.130 | 1.00 | 37.74 |
| ATOM | 4394 | OD1 | ASP | A | 549 | 25.432 | 68.479 | 86.297 | 1.00 | 48.21 |
| ATOM | 4395 | OD2 | ASP | A | 549 | 27.076 | 67.115 | 86.882 | 1.00 | 46.51 |
| ATOM | 4396 | N   | ALA | A | 550 | 23.766 | 64.073 | 84.032 | 1.00 | 27.68 |
| ATOM | 4397 | CA  | ALA | A | 550 | 23.445 | 63.133 | 82.965 | 1.00 | 26.74 |
| ATOM | 4398 | C   | ALA | A | 550 | 22.019 | 63.171 | 82.431 | 1.00 | 32.35 |
| ATOM | 4399 | O   | ALA | A | 550 | 21.745 | 62.615 | 81.361 | 1.00 | 31.95 |
| ATOM | 4400 | CB  | ALA | A | 550 | 23.812 | 61.713 | 83.372 | 1.00 | 25.48 |
| ATOM | 4401 | N   | ILE | A | 551 | 21.123 | 63.795 | 83.192 | 1.00 | 28.71 |
| ATOM | 4402 | CA  | ILE | A | 551 | 19.716 | 63.882 | 82.832 | 1.00 | 28.20 |
| ATOM | 4403 | C   | ILE | A | 551 | 19.461 | 64.355 | 81.411 | 1.00 | 32.04 |
| ATOM | 4404 | O   | ILE | A | 551 | 18.833 | 63.679 | 80.619 | 1.00 | 31.75 |
| ATOM | 4405 | CB  | ILE | A | 551 | 18.876 | 64.641 | 83.868 | 1.00 | 30.29 |
| ATOM | 4406 | CG1 | ILE | A | 551 | 19.038 | 63.985 | 85.226 | 1.00 | 31.50 |
| ATOM | 4407 | CG2 | ILE | A | 551 | 17.391 | 64.661 | 83.475 | 1.00 | 24.75 |
| ATOM | 4408 | CD1 | ILE | A | 551 | 18.072 | 64.561 | 86.253 | 1.00 | 31.62 |
| ATOM | 4409 | N   | PRO | A | 552 | 19.969 | 65.529 | 81.099 | 1.00 | 33.75 |
| ATOM | 4410 | CA  | PRO | A | 552 | 19.793 | 66.121 | 79.796 | 1.00 | 32.60 |
| ATOM | 4411 | C   | PRO | A | 552 | 20.240 | 65.224 | 78.669 | 1.00 | 30.34 |
| ATOM | 4412 | O   | PRO | A | 552 | 19.583 | 65.119 | 77.622 | 1.00 | 27.23 |
| ATOM | 4413 | CB  | PRO | A | 552 | 20.659 | 67.383 | 79.787 | 1.00 | 34.45 |
| ATOM | 4414 | CG  | PRO | A | 552 | 21.348 | 67.500 | 81.139 | 1.00 | 38.39 |
| ATOM | 4415 | CD  | PRO | A | 552 | 20.934 | 66.296 | 81.950 | 1.00 | 34.48 |
| ATOM | 4416 | N   | LEU | A | 553 | 21.391 | 64.616 | 78.891 | 1.00 | 23.74 |
| ATOM | 4417 | CA  | LEU | A | 553 | 21.997 | 63.727 | 77.931 | 1.00 | 22.72 |
| ATOM | 4418 | C   | LEU | A | 553 | 21.138 | 62.522 | 77.670 | 1.00 | 32.68 |
| ATOM | 4419 | O   | LEU | A | 553 | 21.015 | 62.087 | 76.523 | 1.00 | 35.70 |
| ATOM | 4420 | CB  | LEU | A | 553 | 23.362 | 63.281 | 78.439 | 1.00 | 21.57 |
| ATOM | 4421 | CG  | LEU | A | 553 | 24.196 | 64.496 | 78.818 | 1.00 | 24.02 |
| ATOM | 4422 | CD1 | LEU | A | 553 | 25.608 | 64.071 | 79.174 | 1.00 | 19.59 |
| ATOM | 4423 | CD2 | LEU | A | 553 | 24.188 | 65.479 | 77.630 | 1.00 | 18.60 |
| ATOM | 4424 | N   | ALA | A | 554 | 20.563 | 61.973 | 78.754 | 1.00 | 30.05 |
| ATOM | 4425 | CA  | ALA | A | 554 | 19.726 | 60.779 | 78.669 | 1.00 | 27.72 |
| ATOM | 4426 | C   | ALA | A | 554 | 18.432 | 61.107 | 77.988 | 1.00 | 36.03 |
| ATOM | 4427 | O   | ALA | A | 554 | 17.944 | 60.332 | 77.163 | 1.00 | 37.08 |
| ATOM | 4428 | CB  | ALA | A | 554 | 19.475 | 60.165 | 80.017 | 1.00 | 26.78 |
| ATOM | 4429 | N   | LEU | A | 555 | 17.898 | 62.283 |        |      |       |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 4445 | NZ  | LYS | A | 556 | 23.239 | 65.661 | 71.401 | 1.00 | 73.00 |
| ATOM | 4446 | N   | MET | A | 557 | 19.154 | 61.623 | 74.248 | 1.00 | 26.96 |
| ATOM | 4447 | CA  | MET | A | 557 | 19.305 | 60.364 | 73.514 | 1.00 | 23.97 |
| ATOM | 4448 | C   | MET | A | 557 | 18.033 | 59.553 | 73.287 | 1.00 | 30.96 |
| ATOM | 4449 | O   | MET | A | 557 | 17.811 | 58.907 | 72.263 | 1.00 | 23.24 |
| ATOM | 4450 | CB  | MET | A | 557 | 20.401 | 59.488 | 74.104 | 1.00 | 24.89 |
| ATOM | 4451 | CG  | MET | A | 557 | 20.533 | 58.163 | 73.368 | 1.00 | 29.37 |
| ATOM | 4452 | SD  | MET | A | 557 | 22.029 | 57.276 | 73.864 | 1.00 | 33.21 |
| ATOM | 4453 | CE  | MET | A | 557 | 21.939 | 55.812 | 72.793 | 1.00 | 30.16 |
| ATOM | 4454 | N   | ALA | A | 558 | 17.203 | 59.568 | 74.287 | 1.00 | 33.42 |
| ATOM | 4455 | CA  | ALA | A | 558 | 16.000 | 58.816 | 74.194 | 1.00 | 33.03 |
| ATOM | 4456 | C   | ALA | A | 558 | 15.042 | 59.345 | 73.163 | 1.00 | 38.12 |
| ATOM | 4457 | O   | ALA | A | 558 | 14.349 | 58.568 | 72.543 | 1.00 | 37.09 |
| ATOM | 4458 | CB  | ALA | A | 558 | 15.317 | 58.780 | 75.553 | 1.00 | 32.89 |
| ATOM | 4459 | N   | THR | A | 559 | 14.994 | 60.665 | 73.032 | 1.00 | 36.76 |
| ATOM | 4460 | CA  | THR | A | 559 | 14.067 | 61.326 | 72.144 | 1.00 | 36.43 |
| ATOM | 4461 | C   | THR | A | 559 | 14.588 | 61.590 | 70.794 | 1.00 | 41.71 |
| ATOM | 4462 | O   | THR | A | 559 | 13.788 | 61.768 | 69.891 | 1.00 | 44.66 |
| ATOM | 4463 | CB  | THR | A | 559 | 13.615 | 62.705 | 72.694 | 1.00 | 43.70 |
| ATOM | 4464 | OG1 | THR | A | 559 | 14.728 | 63.545 | 72.957 | 1.00 | 38.88 |
| ATOM | 4465 | CG2 | THR | A | 559 | 12.764 | 62.549 | 73.942 | 1.00 | 44.95 |
| ATOM | 4466 | N   | GLU | A | 560 | 15.897 | 61.695 | 70.674 | 1.00 | 37.38 |
| ATOM | 4467 | CA  | GLU | A | 560 | 16.495 | 62.018 | 69.395 | 1.00 | 36.51 |
| ATOM | 4468 | C   | GLU | A | 560 | 16.652 | 60.846 | 68.448 | 1.00 | 40.11 |
| ATOM | 4469 | O   | GLU | A | 560 | 17.003 | 61.052 | 67.300 | 1.00 | 43.23 |
| ATOM | 4470 | CB  | GLU | A | 560 | 17.799 | 62.820 | 69.519 | 1.00 | 38.13 |
| ATOM | 4471 | CG  | GLU | A | 560 | 17.653 | 64.142 | 70.292 | 1.00 | 54.29 |
| ATOM | 4472 | CD  | GLU | A | 560 | 18.857 | 65.043 | 70.127 | 1.00 | 78.42 |
| ATOM | 4473 | OE1 | GLU | A | 560 | 19.960 | 64.639 | 69.812 | 1.00 | 32.69 |
| ATOM | 4474 | OE2 | GLU | A | 560 | 18.593 | 66.303 | 70.380 | 1.00 | 85.90 |
| ATOM | 4475 | N   | GLN | A | 561 | 16.425 | 59.627 | 68.955 | 1.00 | 30.45 |
| ATOM | 4476 | CA  | GLN | A | 561 | 16.467 | 58.356 | 68.230 | 1.00 | 22.57 |
| ATOM | 4477 | C   | GLN | A | 561 | 15.398 | 57.523 | 68.878 | 1.00 | 26.95 |
| ATOM | 4478 | O   | GLN | A | 561 | 14.978 | 57.814 | 69.975 | 1.00 | 27.79 |
| ATOM | 4479 | CB  | GLN | A | 561 | 17.829 | 57.661 | 68.128 | 1.00 | 20.64 |
| ATOM | 4480 | CG  | GLN | A | 561 | 18.470 | 57.290 | 69.491 | 1.00 | 22.59 |
| ATOM | 4481 | CD  | GLN | A | 561 | 17.802 | 56.121 | 70.184 | 1.00 | 28.22 |
| ATOM | 4482 | OE1 | GLN | A | 561 | 17.524 | 56.156 | 71.400 | 1.00 | 37.44 |
| ATOM | 4483 | NE2 | GLN | A | 561 | 17.556 | 55.069 | 69.419 | 1.00 | 31.92 |
| ATOM | 4484 | N   | GLY | A | 562 | 14.888 | 56.535 | 68.209 | 1.00 | 26.16 |
| ATOM | 4485 | CA  | GLY | A | 562 | 13.801 | 55.810 | 68.858 | 1.00 | 27.83 |
| ATOM | 4486 | C   | GLY | A | 562 | 13.932 | 54.320 | 68.761 | 1.00 | 41.56 |
| ATOM | 4487 | O   | GLY | A | 562 | 12.936 | 53.614 | 68.677 | 1.00 | 45.37 |
| ATOM | 4488 | N   | ARG | A | 563 | 15.171 | 53.864 | 68.742 | 1.00 | 37.40 |
| ATOM | 4489 | CA  | ARG | A | 563 | 15.457 | 52.453 | 68.689 | 1.00 | 34.41 |
| ATOM | 4490 | C   | ARG | A | 563 | 15.121 | 51.939 | 70.109 | 1.00 | 39.48 |
| ATOM | 4491 | O   | ARG | A | 563 | 15.832 | 52.221 | 71.087 | 1.00 | 40.29 |
| ATOM | 4492 | CB  | ARG | A | 563 | 16.932 | 52.231 | 68.284 | 1.00 | 18.23 |
| ATOM | 4493 | CG  | ARG | A | 563 | 17.309 | 50.755 | 68.169 | 1.00 | 20.07 |
| ATOM | 4494 | CD  | ARG | A | 563 | 18.779 | 50.514 | 68.512 | 1.00 | 25.07 |
| ATOM | 4495 | NE  | ARG | A | 563 | 19.234 | 49.139 | 68.320 | 1.00 | 25.66 |
| ATOM | 4496 | CZ  | ARG | A | 563 | 20.425 | 48.891 | 67.821 | 1.00 | 26.35 |
| ATOM | 4497 | NH1 | ARG | A | 563 | 21.257 | 49.860 | 67.430 | 1.00 | 12.96 |
| ATOM | 4498 | NH2 | ARG | A | 563 | 20.804 | 47.636 | 67.656 | 1.00 | 30.31 |
| ATOM | 4499 | N   | MET | A | 564 | 13.989 | 51.228 | 70.239 | 1.00 | 33.12 |
| ATOM | 4500 | CA  | MET | A | 564 | 13.487 | 50.695 | 71.526 | 1.00 | 31.84 |
| ATOM | 4501 | C   | MET | A | 564 | 14.565 | 50.247 | 72.532 | 1.00 | 31.42 |
| ATOM | 4502 | O   | MET | A | 564 | 14.494 | 50.501 | 73.744 | 1.00 | 25.72 |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 4503 | CB  | MET | A | 564 | 12.323 | 49.682 | 71.365 | 1.00 | 32.45 |
| ATOM | 4504 | CG  | MET | A | 564 | 11.196 | 50.225 | 70.487 | 1.00 | 35.78 |
| ATOM | 4505 | SD  | MET | A | 564 | 9.695  | 49.205 | 70.533 | 1.00 | 40.85 |
| ATOM | 4506 | CE  | MET | A | 564 | 10.177 | 47.892 | 69.382 | 1.00 | 35.87 |
| ATOM | 4507 | N   | LYS | A | 565 | 15.562 | 49.581 | 71.966 | 1.00 | 31.68 |
| ATOM | 4508 | CA  | LYS | A | 565 | 16.699 | 49.041 | 72.668 | 1.00 | 29.04 |
| ATOM | 4509 | C   | LYS | A | 565 | 17.281 | 50.089 | 73.562 | 1.00 | 26.36 |
| ATOM | 4510 | O   | LYS | A | 565 | 17.648 | 49.782 | 74.673 | 1.00 | 21.19 |
| ATOM | 4511 | CB  | LYS | A | 565 | 17.747 | 48.494 | 71.697 | 1.00 | 29.06 |
| ATOM | 4512 | CG  | LYS | A | 565 | 18.864 | 47.715 | 72.359 | 1.00 | 23.89 |
| ATOM | 4513 | CD  | LYS | A | 565 | 19.982 | 47.355 | 71.392 | 1.00 | 35.75 |
| ATOM | 4514 | CE  | LYS | A | 565 | 20.796 | 46.153 | 71.842 | 1.00 | 36.31 |
| ATOM | 4515 | NZ  | LYS | A | 565 | 22.233 | 46.311 | 71.577 | 1.00 | 44.91 |
| ATOM | 4516 | N   | PHE | A | 566 | 17.321 | 51.321 | 73.073 | 1.00 | 22.91 |
| ATOM | 4517 | CA  | PHE | A | 566 | 17.866 | 52.423 | 73.833 | 1.00 | 24.36 |
| ATOM | 4518 | C   | PHE | A | 566 | 16.814 | 53.253 | 74.571 | 1.00 | 30.37 |
| ATOM | 4519 | O   | PHE | A | 566 | 16.882 | 53.540 | 75.758 | 1.00 | 30.52 |
| ATOM | 4520 | CB  | PHE | A | 566 | 18.622 | 53.355 | 72.857 | 1.00 | 25.26 |
| ATOM | 4521 | CG  | PHE | A | 566 | 19.738 | 52.677 | 72.088 | 1.00 | 24.09 |
| ATOM | 4522 | CD1 | PHE | A | 566 | 20.392 | 51.559 | 72.609 | 1.00 | 23.51 |
| ATOM | 4523 | CD2 | PHE | A | 566 | 20.165 | 53.187 | 70.858 | 1.00 | 24.48 |
| ATOM | 4524 | CE1 | PHE | A | 566 | 21.432 | 50.958 | 71.900 | 1.00 | 23.73 |
| ATOM | 4525 | CE2 | PHE | A | 566 | 21.211 | 52.620 | 70.129 | 1.00 | 24.75 |
| ATOM | 4526 | CZ  | PHE | A | 566 | 21.828 | 51.491 | 70.668 | 1.00 | 25.20 |
| ATOM | 4527 | N   | THR | A | 567 | 15.860 | 53.679 | 73.801 | 1.00 | 31.17 |
| ATOM | 4528 | CA  | THR | A | 567 | 14.783 | 54.533 | 74.239 | 1.00 | 31.74 |
| ATOM | 4529 | C   | THR | A | 567 | 13.985 | 54.037 | 75.458 | 1.00 | 33.79 |
| ATOM | 4530 | O   | THR | A | 567 | 13.657 | 54.818 | 76.373 | 1.00 | 26.01 |
| ATOM | 4531 | CB  | THR | A | 567 | 13.895 | 54.892 | 73.017 | 1.00 | 36.51 |
| ATOM | 4532 | OG1 | THR | A | 567 | 14.527 | 55.844 | 72.138 | 1.00 | 24.12 |
| ATOM | 4533 | CG2 | THR | A | 567 | 12.522 | 55.361 | 73.473 | 1.00 | 34.94 |
| ATOM | 4534 | N   | ARG | A | 568 | 13.663 | 52.726 | 75.469 | 1.00 | 30.74 |
| ATOM | 4535 | CA  | ARG | A | 568 | 12.864 | 52.166 | 76.545 | 1.00 | 26.30 |
| ATOM | 4536 | C   | ARG | A | 568 | 13.486 | 52.226 | 77.882 | 1.00 | 28.61 |
| ATOM | 4537 | O   | ARG | A | 568 | 12.876 | 52.667 | 78.832 | 1.00 | 30.84 |
| ATOM | 4538 | CB  | ARG | A | 568 | 12.315 | 50.798 | 76.251 | 1.00 | 18.11 |
| ATOM | 4539 | CG  | ARG | A | 568 | 11.342 | 50.919 | 75.088 | 1.00 | 29.19 |
| ATOM | 4540 | CD  | ARG | A | 568 | 10.550 | 49.660 | 74.799 | 1.00 | 19.19 |
| ATOM | 4541 | NE  | ARG | A | 568 | 9.707  | 49.343 | 75.917 | 1.00 | 28.72 |
| ATOM | 4542 | CZ  | ARG | A | 568 | 9.254  | 48.138 | 76.133 | 1.00 | 32.39 |
| ATOM | 4543 | NH1 | ARG | A | 568 | 9.528  | 47.144 | 75.291 | 1.00 | 29.79 |
| ATOM | 4544 | NH2 | ARG | A | 568 | 8.507  | 47.930 | 77.208 | 1.00 | 16.44 |
| ATOM | 4545 | N   | PRO | A | 569 | 14.705 | 51.774 |        |      |       |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 4561 | CA  | PHE | A | 571 | 13.084 | 56.541 | 79.758 | 1.00 | 27.27 |
| ATOM | 4562 | C   | PHE | A | 571 | 12.813 | 55.899 | 81.095 | 1.00 | 25.94 |
| ATOM | 4563 | O   | PHE | A | 571 | 12.399 | 56.536 | 82.030 | 1.00 | 27.16 |
| ATOM | 4564 | CB  | PHE | A | 571 | 11.888 | 56.375 | 78.828 | 1.00 | 27.60 |
| ATOM | 4565 | CG  | PHE | A | 571 | 11.546 | 57.616 | 78.042 | 1.00 | 27.70 |
| ATOM | 4566 | CD1 | PHE | A | 571 | 11.193 | 58.820 | 78.651 | 1.00 | 29.97 |
| ATOM | 4567 | CD2 | PHE | A | 571 | 11.557 | 57.570 | 76.651 | 1.00 | 28.87 |
| ATOM | 4568 | CE1 | PHE | A | 571 | 10.861 | 59.953 | 77.910 | 1.00 | 28.24 |
| ATOM | 4569 | CE2 | PHE | A | 571 | 11.233 | 58.684 | 75.886 | 1.00 | 30.43 |
| ATOM | 4570 | CZ  | PHE | A | 571 | 10.877 | 59.875 | 76.520 | 1.00 | 29.55 |
| ATOM | 4571 | N   | LYS | A | 572 | 13.089 | 54.618 | 81.196 | 1.00 | 22.77 |
| ATOM | 4572 | CA  | LYS | A | 572 | 12.845 | 53.946 | 82.468 | 1.00 | 25.43 |
| ATOM | 4573 | C   | LYS | A | 572 | 13.783 | 54.425 | 83.561 | 1.00 | 34.48 |
| ATOM | 4574 | O   | LYS | A | 572 | 13.351 | 54.920 | 84.602 | 1.00 | 35.11 |
| ATOM | 4575 | CB  | LYS | A | 572 | 12.736 | 52.428 | 82.392 | 1.00 | 26.89 |
| ATOM | 4576 | CG  | LYS | A | 572 | 11.303 | 51.911 | 82.326 | 1.00 | 44.03 |
| ATOM | 4577 | CD  | LYS | A | 572 | 11.219 | 50.426 | 81.922 | 1.00 | 57.87 |
| ATOM | 4578 | CE  | LYS | A | 572 | 10.975 | 50.204 | 80.422 | 1.00 | 65.25 |
| ATOM | 4579 | NZ  | LYS | A | 572 | 11.535 | 48.954 | 79.850 | 1.00 | 61.06 |
| ATOM | 4580 | N   | ASP | A | 573 | 15.074 | 54.292 | 83.319 | 1.00 | 31.94 |
| ATOM | 4581 | CA  | ASP | A | 573 | 16.032 | 54.751 | 84.291 | 1.00 | 30.55 |
| ATOM | 4582 | C   | ASP | A | 573 | 15.684 | 56.166 | 84.712 | 1.00 | 32.26 |
| ATOM | 4583 | O   | ASP | A | 573 | 15.693 | 56.453 | 85.895 | 1.00 | 31.85 |
| ATOM | 4584 | CB  | ASP | A | 573 | 17.453 | 54.788 | 83.718 | 1.00 | 32.87 |
| ATOM | 4585 | CG  | ASP | A | 573 | 18.051 | 53.443 | 83.487 | 1.00 | 33.43 |
| ATOM | 4586 | OD1 | ASP | A | 573 | 17.517 | 52.422 | 83.853 | 1.00 | 29.11 |
| ATOM | 4587 | OD2 | ASP | A | 573 | 19.206 | 53.501 | 82.864 | 1.00 | 35.22 |
| ATOM | 4588 | N   | LEU | A | 574 | 15.387 | 57.071 | 83.745 | 1.00 | 29.50 |
| ATOM | 4589 | CA  | LEU | A | 574 | 15.062 | 58.461 | 84.109 | 1.00 | 27.65 |
| ATOM | 4590 | C   | LEU | A | 574 | 13.887 | 58.577 | 85.075 | 1.00 | 32.88 |
| ATOM | 4591 | O   | LEU | A | 574 | 13.864 | 59.411 | 85.962 | 1.00 | 31.04 |
| ATOM | 4592 | CB  | LEU | A | 574 | 14.844 | 59.385 | 82.909 | 1.00 | 26.24 |
| ATOM | 4593 | CG  | LEU | A | 574 | 16.068 | 59.567 | 82.027 | 1.00 | 30.41 |
| ATOM | 4594 | CD1 | LEU | A | 574 | 15.644 | 59.922 | 80.582 | 1.00 | 28.47 |
| ATOM | 4595 | CD2 | LEU | A | 574 | 16.974 | 60.659 | 82.604 | 1.00 | 27.06 |
| ATOM | 4596 | N   | ALA | A | 575 | 12.895 | 57.723 | 84.874 | 1.00 | 32.80 |
| ATOM | 4597 | CA  | ALA | A | 575 | 11.709 | 57.713 | 85.711 | 1.00 | 31.11 |
| ATOM | 4598 | C   | ALA | A | 575 | 12.002 | 57.140 | 87.083 | 1.00 | 35.71 |
| ATOM | 4599 | O   | ALA | A | 575 | 11.309 | 57.362 | 88.055 | 1.00 | 39.91 |
| ATOM | 4600 | CB  | ALA | A | 575 | 10.631 | 56.890 | 85.024 | 1.00 | 30.56 |
| ATOM | 4601 | N   | ALA | A | 576 | 13.049 | 56.364 | 87.170 | 1.00 | 28.55 |
| ATOM | 4602 | CA  | ALA | A | 576 | 13.390 | 55.778 | 88.448 | 1.00 | 22.80 |
| ATOM | 4603 | C   | ALA | A | 576 | 14.258 |        |        |      |       |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 4619 | C   | ASP | A | 578 | 13.862 | 62.357 | 90.881 | 1.00 | 28.55 |
| ATOM | 4620 | O   | ASP | A | 578 | 12.877 | 63.004 | 90.599 | 1.00 | 32.65 |
| ATOM | 4621 | CB  | ASP | A | 578 | 13.804 | 61.192 | 93.055 | 1.00 | 32.60 |
| ATOM | 4622 | CG  | ASP | A | 578 | 15.153 | 61.647 | 93.550 | 1.00 | 53.21 |
| ATOM | 4623 | OD1 | ASP | A | 578 | 16.175 | 61.594 | 92.872 | 1.00 | 51.81 |
| ATOM | 4624 | OD2 | ASP | A | 578 | 15.104 | 62.072 | 94.796 | 1.00 | 64.93 |
| ATOM | 4625 | N   | LYS | A | 579 | 15.104 | 62.750 | 90.674 | 1.00 | 20.12 |
| ATOM | 4626 | CA  | LYS | A | 579 | 15.470 | 64.012 | 90.084 | 1.00 | 21.01 |
| ATOM | 4627 | C   | LYS | A | 579 | 14.934 | 64.270 | 88.697 | 1.00 | 30.25 |
| ATOM | 4628 | O   | LYS | A | 579 | 14.620 | 65.413 | 88.368 | 1.00 | 35.12 |
| ATOM | 4629 | CB  | LYS | A | 579 | 16.982 | 64.223 | 90.104 | 1.00 | 24.11 |
| ATOM | 4630 | CG  | LYS | A | 579 | 17.552 | 64.202 | 91.512 | 1.00 | 48.98 |
| ATOM | 4631 | CD  | LYS | A | 579 | 17.252 | 65.488 | 92.286 | 1.00 | 76.92 |
| ATOM | 4632 | CE  | LYS | A | 579 | 16.495 | 65.258 | 93.588 | 1.00 | 87.93 |
| ATOM | 4633 | NZ  | LYS | A | 579 | 17.282 | 64.550 | 94.611 | 1.00 | 89.56 |
| ATOM | 4634 | N   | SER | A | 580 | 14.838 | 63.244 | 87.857 | 1.00 | 28.66 |
| ATOM | 4635 | CA  | SER | A | 580 | 14.368 | 63.437 | 86.459 | 1.00 | 28.56 |
| ATOM | 4636 | C   | SER | A | 580 | 13.007 | 62.829 | 86.129 | 1.00 | 32.95 |
| ATOM | 4637 | O   | SER | A | 580 | 12.561 | 62.870 | 84.992 | 1.00 | 35.30 |
| ATOM | 4638 | CB  | SER | A | 580 | 15.337 | 62.774 | 85.517 | 1.00 | 25.69 |
| ATOM | 4639 | OG  | SER | A | 580 | 15.476 | 61.424 | 85.969 | 1.00 | 25.12 |
| ATOM | 4640 | N   | HIS | A | 581 | 12.364 | 62.230 | 87.098 | 1.00 | 26.81 |
| ATOM | 4641 | CA  | HIS | A | 581 | 11.100 | 61.595 | 86.850 | 1.00 | 28.26 |
| ATOM | 4642 | C   | HIS | A | 581 | 10.067 | 62.399 | 86.042 | 1.00 | 36.50 |
| ATOM | 4643 | O   | HIS | A | 581 | 9.644  | 62.031 | 84.927 | 1.00 | 34.71 |
| ATOM | 4644 | CB  | HIS | A | 581 | 10.553 | 61.047 | 88.152 | 1.00 | 29.76 |
| ATOM | 4645 | CG  | HIS | A | 581 | 9.148  | 60.588 | 87.968 | 1.00 | 35.31 |
| ATOM | 4646 | ND1 | HIS | A | 581 | 8.111  | 61.494 | 87.899 | 1.00 | 38.92 |
| ATOM | 4647 | CD2 | HIS | A | 581 | 8.634  | 59.338 | 87.891 | 1.00 | 36.84 |
| ATOM | 4648 | CE1 | HIS | A | 581 | 6.999  | 60.783 | 87.817 | 1.00 | 38.85 |
| ATOM | 4649 | NE2 | HIS | A | 581 | 7.280  | 59.488 | 87.734 | 1.00 | 38.13 |
| ATOM | 4650 | N   | ASP | A | 582 | 9.656  | 63.502 | 86.639 | 1.00 | 35.79 |
| ATOM | 4651 | CA  | ASP | A | 582 | 8.680  | 64.388 | 86.064 | 1.00 | 34.39 |
| ATOM | 4652 | C   | ASP | A | 582 | 9.035  | 64.807 | 84.659 | 1.00 | 37.82 |
| ATOM | 4653 | O   | ASP | A | 582 | 8.220  | 64.704 | 83.735 | 1.00 | 37.01 |
| ATOM | 4654 | CB  | ASP | A | 582 | 8.428  | 65.552 | 87.001 | 1.00 | 36.57 |
| ATOM | 4655 | CG  | ASP | A | 582 | 7.597  | 65.110 | 88.167 | 1.00 | 58.09 |
| ATOM | 4656 | OD1 | ASP | A | 582 | 6.708  | 64.289 | 88.070 | 1.00 | 63.17 |
| ATOM | 4657 | OD2 | ASP | A | 582 | 7.920  | 65.708 | 89.279 | 1.00 | 73.96 |
| ATOM | 4658 | N   | GLN | A | 583 | 10.272 | 65.255 | 84.488 | 1.00 | 32.88 |
| ATOM | 4659 | CA  | GLN | A | 583 | 10.750 | 65.648 | 83.169 | 1.00 | 29.92 |
| ATOM | 4660 | C   | GLN | A | 583 | 10.690 | 64.464 | 82.168 | 1.00 | 37.12 |
| ATOM | 4661 | O   | GLN | A | 583 | 10.362 | 64.624 | 80.990 |      |       |



|      |      |               |        |        |        |      |       |
|------|------|---------------|--------|--------|--------|------|-------|
| ATOM | 4677 | CG1 VAL A 585 | 4.959  | 61.947 | 82.955 | 1.00 | 30.03 |
| ATOM | 4678 | CG2 VAL A 585 | 6.464  | 60.085 | 83.539 | 1.00 | 27.82 |
| ATOM | 4679 | N ARG A 586   | 7.000  | 64.123 | 81.333 | 1.00 | 35.76 |
| ATOM | 4680 | CA ARG A 586  | 6.574  | 65.242 | 80.562 | 1.00 | 36.20 |
| ATOM | 4681 | C ARG A 586   | 7.146  | 65.125 | 79.180 | 1.00 | 44.65 |
| ATOM | 4682 | O ARG A 586   | 6.459  | 65.355 | 78.197 | 1.00 | 48.32 |
| ATOM | 4683 | CB ARG A 586  | 7.116  | 66.498 | 81.208 | 1.00 | 38.13 |
| ATOM | 4684 | CG ARG A 586  | 6.744  | 67.799 | 80.518 | 1.00 | 61.01 |
| ATOM | 4685 | CD ARG A 586  | 7.077  | 69.029 | 81.354 | 1.00 | 73.03 |
| ATOM | 4686 | NE ARG A 586  | 8.491  | 69.128 | 81.711 | 1.00 | 86.05 |
| ATOM | 4687 | CZ ARG A 586  | 8.961  | 69.001 | 82.957 | 1.00 | 98.46 |
| ATOM | 4688 | NH1 ARG A 586 | 8.167  | 68.741 | 84.004 | 1.00 | 79.75 |
| ATOM | 4689 | NH2 ARG A 586 | 10.268 | 69.103 | 83.159 | 1.00 | 77.55 |
| ATOM | 4690 | N THR A 587   | 8.426  | 64.769 | 79.110 | 1.00 | 39.49 |
| ATOM | 4691 | CA THR A 587  | 9.099  | 64.646 | 77.822 | 1.00 | 36.80 |
| ATOM | 4692 | C THR A 587   | 8.387  | 63.690 | 76.869 | 1.00 | 37.11 |
| ATOM | 4693 | O THR A 587   | 8.229  | 63.931 | 75.678 | 1.00 | 36.91 |
| ATOM | 4694 | CB THR A 587  | 10.634 | 64.384 | 77.917 | 1.00 | 39.40 |
| ATOM | 4695 | OG1 THR A 587 | 11.303 | 65.334 | 78.717 | 1.00 | 46.27 |
| ATOM | 4696 | CG2 THR A 587 | 11.233 | 64.460 | 76.529 | 1.00 | 32.60 |
| ATOM | 4697 | N TYR A 588   | 7.934  | 62.587 | 77.393 | 1.00 | 33.33 |
| ATOM | 4698 | CA TYR A 588  | 7.252  | 61.639 | 76.555 | 1.00 | 33.94 |
| ATOM | 4699 | C TYR A 588   | 5.890  | 62.146 | 76.090 | 1.00 | 37.02 |
| ATOM | 4700 | O TYR A 588   | 5.428  | 61.880 | 74.988 | 1.00 | 41.55 |
| ATOM | 4701 | CB TYR A 588  | 7.042  | 60.383 | 77.396 | 1.00 | 33.96 |
| ATOM | 4702 | CG TYR A 588  | 6.017  | 59.440 | 76.851 | 1.00 | 33.08 |
| ATOM | 4703 | CD1 TYR A 588 | 6.331  | 58.640 | 75.754 | 1.00 | 35.64 |
| ATOM | 4704 | CD2 TYR A 588 | 4.758  | 59.288 | 77.437 | 1.00 | 34.09 |
| ATOM | 4705 | CE1 TYR A 588 | 5.424  | 57.703 | 75.251 | 1.00 | 34.36 |
| ATOM | 4706 | CE2 TYR A 588 | 3.822  | 58.378 | 76.932 | 1.00 | 34.05 |
| ATOM | 4707 | CZ TYR A 588  | 4.162  | 57.581 | 75.834 | 1.00 | 33.89 |
| ATOM | 4708 | OH TYR A 588  | 3.275  | 56.674 | 75.322 | 1.00 | 23.43 |
| ATOM | 4709 | N GLN A 589   | 5.216  | 62.853 | 76.959 | 1.00 | 25.04 |
| ATOM | 4710 | CA GLN A 589  | 3.914  | 63.339 | 76.612 | 1.00 | 21.41 |
| ATOM | 4711 | C GLN A 589   | 3.992  | 64.304 | 75.481 | 1.00 | 28.78 |
| ATOM | 4712 | O GLN A 589   | 3.099  | 64.410 | 74.678 | 1.00 | 31.24 |
| ATOM | 4713 | CB GLN A 589  | 3.241  | 63.935 | 77.832 | 1.00 | 21.73 |
| ATOM | 4714 | CG GLN A 589  | 2.878  | 62.820 | 78.827 | 1.00 | 22.30 |
| ATOM | 4715 | CD GLN A 589  | 1.695  | 62.069 | 78.293 | 1.00 | 52.83 |
| ATOM | 4716 | OE1 GLN A 589 | 1.511  | 62.003 | 77.075 | 1.00 | 60.15 |
| ATOM | 4717 | NE2 GLN A 589 | 0.864  | 61.542 | 79.182 | 1.00 | 53.04 |
| ATOM | 4718 | N GLU A 590   | 5.099  | 65.001 | 75.409 | 1.00 | 28.36 |
| ATOM | 4719 | CA GLU A 590  | 5.276  | 65.966 | 74.355 | 1.00 | 26.87 |
| ATOM | 4720 | C GLU A 590   | 5.840  | 65.338 | 73.140 | 1.00 | 35.10 |
| ATOM | 4721 | O GLU A 590   | 6.096  | 66.059 | 72.171 | 1.00 | 40.28 |
| ATOM | 4722 | CB GLU A 590  | 6.323  | 67.011 | 74.747 | 1.00 | 27.61 |
| ATOM | 4723 | CG GLU A 590  | 5.846  | 67.954 | 75.847 | 1.00 | 44.11 |
| ATOM | 4724 | CD GLU A 590  | 6.981  | 68.759 | 76.388 | 1.00 | 75.35 |
| ATOM | 4725 | OE1 GLU A 590 | 8.120  | 68.689 | 75.925 | 1.00 | 54.78 |
| ATOM | 4726 | OE2 GLU A 590 | 6.609  | 69.516 | 77.403 | 1.00 | 59.46 |
| ATOM | 4727 | N HIS A 591   | 6.091  | 64.031 | 73.207 | 1.00 | 27.57 |
| ATOM | 4728 | CA HIS A 591  | 6.713  | 63.384 | 72.086 | 1.00 | 25.58 |
| ATOM | 4729 | C HIS A 591   | 5.928  | 62.249 | 71.578 | 1.00 | 32.34 |
| ATOM | 4730 | O HIS A 591   | 6.184  | 61.751 | 70.496 | 1.00 | 38.53 |
| ATOM | 4731 | CB HIS A 591  | 8.094  | 62.851 | 72.487 | 1.00 | 26.32 |
| ATOM | 4732 | CG HIS A 591  | 9.219  | 63.809 | 72.268 | 1.00 | 31.06 |
| ATOM | 4733 | ND1 HIS A 591 | 9.630  | 64.680 | 73.255 | 1.00 | 32.65 |
| ATOM | 4734 | CD2 HIS A 591 | 9.998  | 64.032 | 71.169 | 1.00 | 34.91 |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 4735 | CE1 | HIS | A | 591 | 10.635 | 65.404 | 72.756 | 1.00 | 32.01 |
| ATOM | 4736 | NE2 | HIS | A | 591 | 10.884 | 65.037 | 71.508 | 1.00 | 33.36 |
| ATOM | 4737 | N   | LYS | A | 592 | 4.978  | 61.812 | 72.337 | 1.00 | 28.34 |
| ATOM | 4738 | CA  | LYS | A | 592 | 4.254  | 60.643 | 71.849 | 1.00 | 29.96 |
| ATOM | 4739 | C   | LYS | A | 592 | 3.654  | 60.692 | 70.432 | 1.00 | 33.41 |
| ATOM | 4740 | O   | LYS | A | 592 | 3.819  | 59.769 | 69.592 | 1.00 | 29.05 |
| ATOM | 4741 | CB  | LYS | A | 592 | 3.362  | 59.983 | 72.888 | 1.00 | 32.83 |
| ATOM | 4742 | CG  | LYS | A | 592 | 2.435  | 60.930 | 73.615 | 1.00 | 31.14 |
| ATOM | 4743 | CD  | LYS | A | 592 | 1.677  | 60.203 | 74.704 | 1.00 | 38.97 |
| ATOM | 4744 | CE  | LYS | A | 592 | 0.253  | 60.691 | 74.890 | 1.00 | 25.02 |
| ATOM | 4745 | NZ  | LYS | A | 592 | -0.157 | 60.632 | 76.302 | 1.00 | 45.83 |
| ATOM | 4746 | N   | ALA | A | 593 | 2.934  | 61.782 | 70.187 | 1.00 | 30.97 |
| ATOM | 4747 | CA  | ALA | A | 593 | 2.260  | 62.026 | 68.917 | 1.00 | 28.47 |
| ATOM | 4748 | C   | ALA | A | 593 | 3.169  | 61.943 | 67.703 | 1.00 | 32.66 |
| ATOM | 4749 | O   | ALA | A | 593 | 2.775  | 61.488 | 66.639 | 1.00 | 36.77 |
| ATOM | 4750 | CB  | ALA | A | 593 | 1.571  | 63.379 | 68.954 | 1.00 | 27.35 |
| ATOM | 4751 | N   | SER | A | 594 | 4.384  | 62.405 | 67.869 | 1.00 | 27.08 |
| ATOM | 4752 | CA  | SER | A | 594 | 5.345  | 62.417 | 66.794 | 1.00 | 30.04 |
| ATOM | 4753 | C   | SER | A | 594 | 6.185  | 61.169 | 66.760 | 1.00 | 36.80 |
| ATOM | 4754 | O   | SER | A | 594 | 6.995  | 60.991 | 65.848 | 1.00 | 37.94 |
| ATOM | 4755 | CB  | SER | A | 594 | 6.292  | 63.596 | 66.977 | 1.00 | 37.69 |
| ATOM | 4756 | OG  | SER | A | 594 | 7.199  | 63.340 | 68.043 | 1.00 | 54.55 |
| ATOM | 4757 | N   | MET | A | 595 | 6.015  | 60.340 | 67.776 | 1.00 | 33.12 |
| ATOM | 4758 | CA  | MET | A | 595 | 6.794  | 59.115 | 67.898 | 1.00 | 33.96 |
| ATOM | 4759 | C   | MET | A | 595 | 6.200  | 57.936 | 67.125 | 1.00 | 40.91 |
| ATOM | 4760 | O   | MET | A | 595 | 5.019  | 57.927 | 66.809 | 1.00 | 50.82 |
| ATOM | 4761 | CB  | MET | A | 595 | 6.716  | 58.686 | 69.382 | 1.00 | 34.22 |
| ATOM | 4762 | CG  | MET | A | 595 | 7.621  | 59.371 | 70.399 | 1.00 | 34.61 |
| ATOM | 4763 | SD  | MET | A | 595 | 7.606  | 58.440 | 71.962 | 1.00 | 39.24 |
| ATOM | 4764 | CE  | MET | A | 595 | 7.145  | 59.779 | 73.084 | 1.00 | 36.72 |
| ATOM | 4765 | N   | HIS | A | 596 | 6.987  | 56.897 | 66.886 | 1.00 | 26.19 |
| ATOM | 4766 | CA  | HIS | A | 596 | 6.496  | 55.657 | 66.246 | 1.00 | 23.19 |
| ATOM | 4767 | C   | HIS | A | 596 | 5.438  | 54.964 | 67.120 | 1.00 | 25.21 |
| ATOM | 4768 | O   | HIS | A | 596 | 5.621  | 54.728 | 68.311 | 1.00 | 22.59 |
| ATOM | 4769 | CB  | HIS | A | 596 | 7.657  | 54.655 | 66.077 | 1.00 | 24.41 |
| ATOM | 4770 | CG  | HIS | A | 596 | 7.222  | 53.366 | 65.493 | 1.00 | 30.13 |
| ATOM | 4771 | ND1 | HIS | A | 596 | 7.606  | 52.995 | 64.214 | 1.00 | 32.86 |
| ATOM | 4772 | CD2 | HIS | A | 596 | 6.421  | 52.385 | 66.005 | 1.00 | 30.90 |
| ATOM | 4773 | CE1 | HIS | A | 596 | 7.047  | 51.824 | 63.974 | 1.00 | 30.05 |
| ATOM | 4774 | NE2 | HIS | A | 596 | 6.325  | 51.441 | 65.031 | 1.00 | 30.20 |
| ATOM | 4775 | N   | PRO | A | 597 | 4.334  | 54.587 | 66.512 | 1.00 | 27.08 |
| ATOM | 4776 | CA  | PRO | A | 597 | 3.217  | 53.912 | 67.173 | 1.00 | 26.35 |
| ATOM | 4777 | C   | PRO | A | 597 | 3.513  | 52.851 | 68.248 | 1.00 | 37.51 |
| ATOM | 4778 | O   | PRO | A | 597 | 2.979  | 52.900 | 69.348 | 1.00 | 41.16 |
| ATOM | 4779 | CB  | PRO | A | 597 | 2.334  | 53.307 | 66.076 | 1.00 | 26.17 |
| ATOM | 4780 | CG  | PRO | A | 597 | 3.140  | 53.426 | 64.792 | 1.00 | 34.56 |
| ATOM | 4781 | CD  | PRO | A | 597 | 4.285  | 54.418 | 65.050 | 1.00 | 30.06 |
| ATOM | 4782 | N   | VAL | A | 598 | 4.311  | 51.850 | 67.939 | 1.00 | 33.08 |
| ATOM | 4783 | CA  | VAL | A | 598 | 4.585  | 50.802 | 68.911 | 1.00 | 28.39 |
| ATOM | 4784 | C   | VAL | A | 598 | 5.444  | 51.307 | 70.029 | 1.00 | 29.32 |
| ATOM | 4785 | O   | VAL | A | 598 | 5.168  | 51.096 | 71.217 | 1.00 | 29.13 |
| ATOM | 4786 | CB  | VAL | A | 598 | 5.196  | 49.599 | 68.210 | 1.00 | 27.99 |
| ATOM | 4787 | CG1 | VAL | A | 598 | 5.806  | 48.608 | 69.187 | 1.00 | 26.98 |
| ATOM | 4788 | CG2 | VAL | A | 598 | 4.144  | 48.944 | 67.296 | 1.00 | 26.13 |
| ATOM | 4789 | N   | THR | A | 599 | 6.480  | 52.021 | 69.635 | 1.00 | 26.10 |
| ATOM | 4790 | CA  | THR | A | 599 | 7.370  | 52.573 | 70.631 | 1.00 | 26.95 |
| ATOM | 4791 | C   | THR | A | 599 | 6.650  | 53.404 | 71.669 | 1.00 | 30.81 |
| ATOM | 4792 | O   | THR | A | 599 | 6.863  | 53.327 | 72.871 | 1.00 | 31.33 |



|      |      |     |     |   |     |       |        |        |      |       |
|------|------|-----|-----|---|-----|-------|--------|--------|------|-------|
| ATOM | 4793 | CB  | THR | A | 599 | 8.413 | 53.455 | 69.975 | 1.00 | 26.67 |
| ATOM | 4794 | OG1 | THR | A | 599 | 9.092 | 52.725 | 68.958 | 1.00 | 27.92 |
| ATOM | 4795 | CG2 | THR | A | 599 | 9.358 | 53.884 | 71.092 | 1.00 | 20.69 |
| ATOM | 4796 | N   | ALA | A | 600 | 5.801 | 54.218 | 71.135 | 1.00 | 26.41 |
| ATOM | 4797 | CA  | ALA | A | 600 | 4.997 | 55.111 | 71.878 | 1.00 | 26.39 |
| ATOM | 4798 | C   | ALA | A | 600 | 4.176 | 54.339 | 72.860 | 1.00 | 32.00 |
| ATOM | 4799 | O   | ALA | A | 600 | 4.162 | 54.597 | 74.057 | 1.00 | 35.37 |
| ATOM | 4800 | CB  | ALA | A | 600 | 4.090 | 55.774 | 70.856 | 1.00 | 27.56 |
| ATOM | 4801 | N   | MET | A | 601 | 3.470 | 53.380 | 72.332 | 1.00 | 26.26 |
| ATOM | 4802 | CA  | MET | A | 601 | 2.627 | 52.585 | 73.167 | 1.00 | 26.60 |
| ATOM | 4803 | C   | MET | A | 601 | 3.439 | 51.909 | 74.225 | 1.00 | 25.73 |
| ATOM | 4804 | O   | MET | A | 601 | 3.099 | 51.964 | 75.381 | 1.00 | 25.77 |
| ATOM | 4805 | CB  | MET | A | 601 | 1.752 | 51.625 | 72.353 | 1.00 | 30.49 |
| ATOM | 4806 | CG  | MET | A | 601 | 1.024 | 50.594 | 73.176 | 1.00 | 36.00 |
| ATOM | 4807 | SD  | MET | A | 601 | 2.043 | 49.146 | 73.554 | 1.00 | 42.41 |
| ATOM | 4808 | CE  | MET | A | 601 | 1.693 | 48.128 | 72.111 | 1.00 | 37.75 |
| ATOM | 4809 | N   | LEU | A | 602 | 4.538 | 51.310 | 73.848 | 1.00 | 21.64 |
| ATOM | 4810 | CA  | LEU | A | 602 | 5.339 | 50.671 | 74.873 | 1.00 | 22.59 |
| ATOM | 4811 | C   | LEU | A | 602 | 6.010 | 51.650 | 75.870 | 1.00 | 29.61 |
| ATOM | 4812 | O   | LEU | A | 602 | 6.137 | 51.346 | 77.039 | 1.00 | 27.62 |
| ATOM | 4813 | CB  | LEU | A | 602 | 6.418 | 49.760 | 74.294 | 1.00 | 22.14 |
| ATOM | 4814 | CG  | LEU | A | 602 | 5.916 | 48.529 | 73.575 | 1.00 | 25.78 |
| ATOM | 4815 | CD1 | LEU | A | 602 | 7.021 | 48.087 | 72.609 | 1.00 | 26.02 |
| ATOM | 4816 | CD2 | LEU | A | 602 | 5.651 | 47.445 | 74.613 | 1.00 | 21.01 |
| ATOM | 4817 | N   | VAL | A | 603 | 6.508 | 52.805 | 75.445 | 1.00 | 27.15 |
| ATOM | 4818 | CA  | VAL | A | 603 | 7.145 | 53.684 | 76.413 | 1.00 | 26.39 |
| ATOM | 4819 | C   | VAL | A | 603 | 6.121 | 54.157 | 77.438 | 1.00 | 32.60 |
| ATOM | 4820 | O   | VAL | A | 603 | 6.436 | 54.235 | 78.621 | 1.00 | 35.31 |
| ATOM | 4821 | CB  | VAL | A | 603 | 7.917 | 54.832 | 75.760 | 1.00 | 27.78 |
| ATOM | 4822 | CG1 | VAL | A | 603 | 8.286 | 55.887 | 76.774 | 1.00 | 24.54 |
| ATOM | 4823 | CG2 | VAL | A | 603 | 9.172 | 54.286 | 75.094 | 1.00 | 27.29 |
| ATOM | 4824 | N   | GLY | A | 604 | 4.878 | 54.434 | 76.976 | 1.00 | 27.44 |
| ATOM | 4825 | CA  | GLY | A | 604 | 3.759 | 54.856 | 77.819 | 1.00 | 27.58 |
| ATOM | 4826 | C   | GLY | A | 604 | 3.418 | 53.797 | 78.905 | 1.00 | 37.00 |
| ATOM | 4827 | O   | GLY | A | 604 | 3.088 | 54.102 | 80.072 | 1.00 | 36.56 |
| ATOM | 4828 | N   | LYS | A | 605 | 3.511 | 52.522 | 78.520 | 1.00 | 32.54 |
| ATOM | 4829 | CA  | LYS | A | 605 | 3.250 | 51.415 | 79.459 | 1.00 | 32.17 |
| ATOM | 4830 | C   | LYS | A | 605 | 4.312 | 51.405 | 80.539 | 1.00 | 35.15 |
| ATOM | 4831 | O   | LYS | A | 605 | 4.040 | 51.347 | 81.734 | 1.00 | 33.77 |
| ATOM | 4832 | CB  | LYS | A | 605 | 3.231 | 50.034 | 78.782 | 1.00 | 33.59 |
| ATOM | 4833 | CG  | LYS | A | 605 | 1.837 | 49.438 | 78.576 | 1.00 | 42.45 |
| ATOM | 4834 | CD  | LYS | A | 605 | 1.846 | 48.115 | 77.815 | 1.00 | 60.83 |
| ATOM | 4835 | CE  | LYS | A | 605 | 1.223 | 46.946 | 78.578 | 1.00 | 86.38 |



|      |      |      |     |   |     |         |        |        |      |        |
|------|------|------|-----|---|-----|---------|--------|--------|------|--------|
| ATOM | 4851 | CD1  | LEU | A | 607 | 7.954   | 57.746 | 80.132 | 1.00 | 34.34  |
| ATOM | 4852 | CD2  | LEU | A | 607 | 8.695   | 56.653 | 82.183 | 1.00 | 41.97  |
| ATOM | 4853 | N    | LYS | A | 608 | 3.895   | 54.062 | 82.586 | 1.00 | 45.01  |
| ATOM | 4854 | CA   | LYS | A | 608 | 2.576   | 53.874 | 83.264 | 1.00 | 46.99  |
| ATOM | 4855 | C    | LYS | A | 608 | 1.625   | 55.088 | 83.181 | 1.00 | 51.31  |
| ATOM | 4856 | O    | LYS | A | 608 | 0.988   | 55.467 | 84.151 | 1.00 | 51.35  |
| ATOM | 4857 | CB   | LYS | A | 608 | 2.813   | 53.510 | 84.750 | 1.00 | 50.83  |
| ATOM | 4858 | CG   | LYS | A | 608 | 3.331   | 52.093 | 84.949 | 1.00 | 63.57  |
| ATOM | 4859 | CD   | LYS | A | 608 | 4.405   | 52.019 | 86.031 | 1.00 | 77.03  |
| ATOM | 4860 | CE   | LYS | A | 608 | 5.341   | 50.825 | 85.858 | 1.00 | 96.44  |
| ATOM | 4861 | NZ   | LYS | A | 608 | 6.034   | 50.554 | 87.117 | 1.00 | 100.00 |
| ATOM | 4862 | N    | VAL | A | 609 | 1.560   | 55.724 | 81.991 | 1.00 | 50.28  |
| ATOM | 4863 | CA   | VAL | A | 609 | 0.688   | 56.901 | 81.852 | 1.00 | 50.89  |
| ATOM | 4864 | C    | VAL | A | 609 | -0.494  | 56.660 | 80.897 | 1.00 | 60.23  |
| ATOM | 4865 | O    | VAL | A | 609 | -1.640  | 56.952 | 81.194 | 1.00 | 63.02  |
| ATOM | 4866 | CB   | VAL | A | 609 | 1.533   | 58.091 | 81.364 | 1.00 | 54.72  |
| ATOM | 4867 | CG1  | VAL | A | 609 | 1.996   | 58.926 | 82.551 | 1.00 | 54.87  |
| ATOM | 4868 | CG2  | VAL | A | 609 | 2.744   | 57.607 | 80.605 | 1.00 | 54.46  |
| ATOM | 4869 | N    | ASP | A | 610 | -0.177  | 56.152 | 79.687 | 1.00 | 58.84  |
| ATOM | 4870 | CA   | ASP | A | 610 | -1.238  | 55.949 | 78.699 | 1.00 | 99.84  |
| ATOM | 4871 | C    | ASP | A | 610 | -2.062  | 54.695 | 79.001 | 1.00 | 100.00 |
| ATOM | 4872 | O    | ASP | A | 610 | -3.247  | 54.615 | 78.711 | 1.00 | 69.75  |
| ATOM | 4873 | CB   | ASP | A | 610 | -0.594  | 55.818 | 77.316 | 1.00 | 100.00 |
| ATOM | 4874 | CG   | ASP | A | 610 | -0.637  | 57.161 | 76.610 | 1.00 | 92.61  |
| ATOM | 4875 | OD1  | ASP | A | 610 | -1.449  | 57.999 | 77.018 | 1.00 | 90.49  |
| ATOM | 4876 | OD2  | ASP | A | 610 | 0.134   | 57.355 | 75.670 | 1.00 | 89.29  |
| ATOM | 4877 | ZN2+ | ZN  | Z | 1   | 17.003  | 38.803 | 64.180 | 1.00 | 28.37  |
| ATOM | 4878 | YB3+ | YB  | Y | 1   | 43.011  | 51.068 | 98.864 | 1.00 | 34.70  |
| ATOM | 4879 | YB3+ | YB  | Y | 2   | -13.786 | 56.771 | 52.040 | 0.50 | 57.25  |
| ATOM | 4880 | YB3+ | YB  | Y | 3   | -10.537 | 57.860 | 52.381 | 0.50 | 36.57  |
| ATOM | 4881 | CG   | IMD | I | 1   | 26.249  | 42.039 | 80.754 | 1.00 | 28.44  |
| ATOM | 4882 | ND1  | IMD | I | 1   | 26.057  | 42.254 | 79.400 | 1.00 | 28.35  |
| ATOM | 4883 | CD2  | IMD | I | 1   | 27.562  | 41.726 | 80.902 | 1.00 | 17.99  |
| ATOM | 4884 | CE1  | IMD | I | 1   | 27.201  | 42.063 | 78.760 | 1.00 | 29.77  |
| ATOM | 4885 | NE2  | IMD | I | 1   | 28.130  | 41.745 | 79.647 | 1.00 | 35.02  |
| ATOM | 4886 | CB   | ACE | C | 1   | 13.616  | 12.333 | 68.475 | 1.00 | 59.33  |
| ATOM | 4887 | CG   | ACE | C | 1   | 12.871  | 13.331 | 69.306 | 1.00 | 42.98  |
| ATOM | 4888 | OD1  | ACE | C | 1   | 12.958  | 14.536 | 69.146 | 1.00 | 39.66  |
| ATOM | 4889 | OD2  | ACE | C | 1   | 12.142  | 12.759 | 70.236 | 1.00 | 47.21  |
| ATOM | 4890 | C6   | INH | V | 1   | 7.422   | 38.514 | 70.154 | 1.00 | 38.70  |
| ATOM | 4891 | C5   | INH | V | 1   | 7.571   | 39.820 | 69.689 | 1.00 | 37.05  |
| ATOM | 4892 | C4   | INH | V | 1   | 7.901   | 40.062 | 68.354 | 1.00 | 31.41  |
| ATOM | 4893 | C3   | INH | V | 1   | 8.091   | 38.967 | 67.505 | 1.00 | 35.48  |



|      |      |   |     |   |    |         |        |         |      |       |
|------|------|---|-----|---|----|---------|--------|---------|------|-------|
| ATOM | 4909 | O | HOH | W | 1  | 44.463  | 49.888 | 77.523  | 1.00 | 46.91 |
| ATOM | 4910 | O | HOH | W | 2  | 13.469  | 27.803 | 78.018  | 1.00 | 20.07 |
| ATOM | 4911 | O | HOH | W | 3  | 4.225   | 69.721 | 58.393  | 1.00 | 27.76 |
| ATOM | 4912 | O | HOH | W | 4  | 15.603  | 28.826 | 61.823  | 1.00 | 22.81 |
| ATOM | 4913 | O | HOH | W | 5  | 22.862  | 26.624 | 42.874  | 1.00 | 53.05 |
| ATOM | 4914 | O | HOH | W | 6  | 8.423   | 46.452 | 57.584  | 1.00 | 32.22 |
| ATOM | 4915 | O | HOH | W | 7  | 17.904  | 46.550 | 68.524  | 1.00 | 31.91 |
| ATOM | 4916 | O | HOH | W | 8  | 22.979  | 45.895 | 83.716  | 1.00 | 39.37 |
| ATOM | 4917 | O | HOH | W | 9  | 17.707  | 39.158 | 55.643  | 1.00 | 25.27 |
| ATOM | 4918 | O | HOH | W | 10 | 12.439  | 36.303 | 59.209  | 1.00 | 31.46 |
| ATOM | 4919 | O | HOH | W | 11 | 17.367  | 62.730 | 50.320  | 1.00 | 37.74 |
| ATOM | 4920 | O | HOH | W | 12 | 42.823  | 52.642 | 90.552  | 1.00 | 53.80 |
| ATOM | 4921 | O | HOH | W | 13 | 34.337  | 45.508 | 97.419  | 1.00 | 57.99 |
| ATOM | 4922 | O | HOH | W | 14 | 6.726   | 27.119 | 48.459  | 1.00 | 62.29 |
| ATOM | 4923 | O | HOH | W | 15 | -0.093  | 30.159 | 71.746  | 1.00 | 29.96 |
| ATOM | 4924 | O | HOH | W | 16 | -19.673 | 44.016 | 58.682  | 1.00 | 58.64 |
| ATOM | 4925 | O | HOH | W | 17 | 16.563  | 26.790 | 80.837  | 1.00 | 38.62 |
| ATOM | 4926 | O | HOH | W | 18 | 10.281  | 35.677 | 88.518  | 1.00 | 26.01 |
| ATOM | 4927 | O | HOH | W | 19 | 20.973  | 35.691 | 44.774  | 1.00 | 49.50 |
| ATOM | 4928 | O | HOH | W | 20 | 0.996   | 19.571 | 53.713  | 1.00 | 67.39 |
| ATOM | 4929 | O | HOH | W | 21 | 20.424  | 37.014 | 85.845  | 1.00 | 39.54 |
| ATOM | 4930 | O | HOH | W | 22 | -2.498  | 35.905 | 53.781  | 1.00 | 51.70 |
| ATOM | 4931 | O | HOH | W | 23 | 39.807  | 49.718 | 92.595  | 1.00 | 37.39 |
| ATOM | 4932 | O | HOH | W | 24 | 16.431  | 58.267 | 93.127  | 1.00 | 47.45 |
| ATOM | 4933 | O | HOH | W | 25 | 6.935   | 45.104 | 66.012  | 1.00 | 18.12 |
| ATOM | 4934 | O | HOH | W | 26 | 40.479  | 54.713 | 100.253 | 1.00 | 28.72 |
| ATOM | 4935 | O | HOH | W | 27 | 22.369  | 40.324 | 67.919  | 1.00 | 46.36 |
| ATOM | 4936 | O | HOH | W | 28 | 37.289  | 49.457 | 68.016  | 1.00 | 61.37 |
| ATOM | 4937 | O | HOH | W | 29 | 2.611   | 35.015 | 55.709  | 1.00 | 24.45 |
| ATOM | 4938 | O | HOH | W | 30 | 41.088  | 62.590 | 98.644  | 1.00 | 65.38 |
| ATOM | 4939 | O | HOH | W | 31 | 17.369  | 55.024 | 87.465  | 1.00 | 24.22 |
| ATOM | 4940 | O | HOH | W | 32 | 25.433  | 20.198 | 55.692  | 1.00 | 44.61 |
| ATOM | 4941 | O | HOH | W | 33 | 3.890   | 42.770 | 66.651  | 1.00 | 22.34 |
| ATOM | 4942 | O | HOH | W | 34 | 3.934   | 63.391 | 62.592  | 1.00 | 60.69 |
| ATOM | 4943 | O | HOH | W | 35 | 22.280  | 41.610 | 86.289  | 1.00 | 74.20 |
| ATOM | 4944 | O | HOH | W | 36 | 22.631  | 46.401 | 90.078  | 1.00 | 47.44 |
| ATOM | 4945 | O | HOH | W | 37 | 33.442  | 20.227 | 64.569  | 1.00 | 55.41 |
| ATOM | 4946 | O | HOH | W | 38 | 39.834  | 28.974 | 75.602  | 1.00 | 41.72 |
| ATOM | 4947 | O | HOH | W | 39 | 35.232  | 47.140 | 54.186  | 1.00 | 37.08 |
| ATOM | 4948 | O | HOH | W | 40 | 36.003  | 57.784 | 57.893  | 1.00 | 43.05 |
| ATOM | 4949 | O | HOH | W | 41 | 37.216  | 27.438 | 74.564  | 1.00 | 50.79 |
| ATOM | 4950 | O | HOH | W | 42 | 17.770  | 67.012 | 77.183  | 1.00 | 45.78 |
| ATOM | 4951 | O | HOH | W | 43 | 5.341   | 31.286 | 78.127  | 1.00 | 25.34 |
| ATOM | 4952 | O | HOH | W | 44 | 33.535  | 32.503 | 52.063  | 1.00 | 56.13 |
| ATOM | 4953 | O | HOH | W | 45 | 25.477  | 33.146 | 44.610  | 1.00 | 65.43 |
| ATOM | 4954 | O | HOH | W | 46 | 16.235  | 37.438 | 52.628  | 1.00 | 32.10 |
| ATOM | 4955 | O | HOH | W | 47 | 28.791  | 14.101 | 63.316  | 1.00 | 46.67 |
| ATOM | 4956 | O | HOH | W | 48 | 10.230  | 24.992 | 86.967  | 1.00 | 38.63 |
| ATOM | 4957 | O | HOH | W | 49 | 30.821  | 38.856 | 79.630  | 1.00 | 40.44 |
| ATOM | 4958 | O | HOH | W | 50 | 12.621  | 37.226 | 62.944  | 1.00 | 26.70 |
| ATOM | 4959 | O | HOH | W | 51 | 27.987  | 30.609 | 66.612  | 1.00 | 33.55 |
| ATOM | 4960 | O | HOH | W | 52 | 34.459  | 28.696 | 64.242  | 1.00 | 51.01 |
| ATOM | 4961 | O | HOH | W | 53 | 34.969  | 62.270 | 91.179  | 1.00 | 68.20 |
| ATOM | 4962 | O | HOH | W | 54 | 33.631  | 30.717 | 62.396  | 1.00 | 41.64 |
| ATOM | 4963 | O | HOH | W | 55 | 43.987  | 48.530 | 91.269  | 1.00 | 50.99 |
| ATOM | 4964 | O | HOH | W | 56 | 23.412  | 28.584 | 85.186  | 1.00 | 69.23 |
| ATOM | 4965 | O | HOH | W | 57 | 39.834  | 28.057 | 72.257  | 1.00 | 81.00 |
| ATOM | 4966 | O | HOH | W | 58 | 2.892   | 25.685 | 69.907  | 1.00 | 38.96 |



|      |      |   |     |   |     |         |        |        |      |       |
|------|------|---|-----|---|-----|---------|--------|--------|------|-------|
| ATOM | 4967 | O | HOH | W | 59  | 10.284  | 47.120 | 72.671 | 1.00 | 40.28 |
| ATOM | 4968 | O | HOH | W | 60  | 32.645  | 39.037 | 76.746 | 1.00 | 21.71 |
| ATOM | 4969 | O | HOH | W | 61  | 43.535  | 48.019 | 95.228 | 1.00 | 37.69 |
| ATOM | 4970 | O | HOH | W | 62  | 11.991  | 51.053 | 43.479 | 1.00 | 41.05 |
| ATOM | 4971 | O | HOH | W | 63  | 18.329  | 56.527 | 89.388 | 1.00 | 28.51 |
| ATOM | 4972 | O | HOH | W | 64  | 16.555  | 9.309  | 68.875 | 1.00 | 89.05 |
| ATOM | 4973 | O | HOH | W | 65  | 23.741  | 44.759 | 73.150 | 1.00 | 38.43 |
| ATOM | 4974 | O | HOH | W | 66  | 19.093  | 53.805 | 41.239 | 1.00 | 55.25 |
| ATOM | 4975 | O | HOH | W | 67  | 31.750  | 60.369 | 56.933 | 1.00 | 92.26 |
| ATOM | 4976 | O | HOH | W | 68  | 24.836  | 68.428 | 80.926 | 1.00 | 59.25 |
| ATOM | 4977 | O | HOH | W | 69  | -21.014 | 19.446 | 48.342 | 1.00 | 52.24 |
| ATOM | 4978 | O | HOH | W | 70  | 11.318  | 68.028 | 86.566 | 1.00 | 77.81 |
| ATOM | 4979 | O | HOH | W | 71  | 5.312   | 60.076 | 63.511 | 1.00 | 36.83 |
| ATOM | 4980 | O | HOH | W | 72  | 7.689   | 20.219 | 84.680 | 1.00 | 32.24 |
| ATOM | 4981 | O | HOH | W | 73  | 34.988  | 44.708 | 64.746 | 1.00 | 40.73 |
| ATOM | 4982 | O | HOH | W | 74  | 10.614  | 49.644 | 41.337 | 1.00 | 38.90 |
| ATOM | 4983 | O | HOH | W | 75  | 19.349  | 42.973 | 64.739 | 1.00 | 54.53 |
| ATOM | 4984 | O | HOH | W | 76  | 35.916  | 30.862 | 80.753 | 1.00 | 55.38 |
| ATOM | 4985 | O | HOH | W | 77  | 9.666   | 26.046 | 46.603 | 1.00 | 40.09 |
| ATOM | 4986 | O | HOH | W | 78  | -10.171 | 46.751 | 60.237 | 1.00 | 29.78 |
| ATOM | 4987 | O | HOH | W | 79  | 46.751  | 58.883 | 86.875 | 1.00 | 35.92 |
| ATOM | 4988 | O | HOH | W | 80  | 19.320  | 32.528 | 51.000 | 1.00 | 33.36 |
| ATOM | 4989 | O | HOH | W | 81  | 28.815  | 39.568 | 66.176 | 1.00 | 59.19 |
| ATOM | 4990 | O | HOH | W | 82  | 38.207  | 35.773 | 73.585 | 1.00 | 17.81 |
| ATOM | 4991 | O | HOH | W | 83  | 23.802  | 33.925 | 75.175 | 1.00 | 25.19 |
| ATOM | 4992 | O | HOH | W | 84  | 42.241  | 51.290 | 99.896 | 1.00 | 15.88 |
| ATOM | 4993 | O | HOH | W | 85  | 3.751   | 36.678 | 58.842 | 1.00 | 24.97 |
| ATOM | 4994 | O | HOH | W | 86  | -7.009  | 40.341 | 62.580 | 1.00 | 25.39 |
| ATOM | 4995 | O | HOH | W | 87  | 11.735  | 58.910 | 68.155 | 1.00 | 39.70 |
| ATOM | 4996 | O | HOH | W | 88  | 13.986  | 52.835 | 42.224 | 1.00 | 50.91 |
| ATOM | 4997 | O | HOH | W | 89  | 1.452   | 46.541 | 69.459 | 1.00 | 35.03 |
| ATOM | 4998 | O | HOH | W | 90  | -1.938  | 55.310 | 56.971 | 1.00 | 28.10 |
| ATOM | 4999 | O | HOH | W | 91  | 13.801  | 66.947 | 52.600 | 1.00 | 38.65 |
| ATOM | 5000 | O | HOH | W | 92  | 21.594  | 47.218 | 79.203 | 1.00 | 30.31 |
| ATOM | 5001 | O | HOH | W | 93  | 10.639  | 58.632 | 90.827 | 1.00 | 43.78 |
| ATOM | 5002 | O | HOH | W | 94  | 33.335  | 53.550 | 68.086 | 1.00 | 37.04 |
| ATOM | 5003 | O | HOH | W | 95  | -1.984  | 28.738 | 60.212 | 1.00 | 31.56 |
| ATOM | 5004 | O | HOH | W | 96  | -4.958  | 51.055 | 59.250 | 1.00 | 34.00 |
| ATOM | 5005 | O | HOH | W | 97  | 17.610  | 39.701 | 51.503 | 1.00 | 28.27 |
| ATOM | 5006 | O | HOH | W | 98  | 10.686  | 54.166 | 67.565 | 1.00 | 37.68 |
| ATOM | 5007 | O | HOH | W | 99  | 20.567  | 43.859 | 78.621 | 1.00 | 41.57 |
| ATOM | 5008 | O | HOH | W | 100 | 7.013   | 22.332 | 69.109 | 1.00 | 28.72 |
| ATOM | 5009 | O | HOH | W | 101 | 10.097  | 53.225 | 78.47  |      |       |



|      |      |   |     |   |     |         |        |        |      |       |
|------|------|---|-----|---|-----|---------|--------|--------|------|-------|
| ATOM | 5025 | O | HOH | W | 117 | 11.870  | 38.304 | 43.174 | 1.00 | 40.85 |
| ATOM | 5026 | O | HOH | W | 118 | -13.844 | 25.597 | 58.258 | 1.00 | 53.75 |
| ATOM | 5027 | O | HOH | W | 119 | 2.929   | 41.135 | 59.858 | 1.00 | 36.49 |
| ATOM | 5028 | O | HOH | W | 120 | 24.890  | 45.490 | 82.167 | 1.00 | 41.65 |
| ATOM | 5029 | O | HOH | W | 121 | 36.062  | 59.335 | 75.090 | 1.00 | 38.82 |
| ATOM | 5030 | O | HOH | W | 122 | -10.715 | 32.037 | 61.699 | 1.00 | 78.82 |
| ATOM | 5031 | O | HOH | W | 123 | -2.646  | 25.492 | 60.812 | 1.00 | 48.40 |
| ATOM | 5032 | O | HOH | W | 124 | -8.948  | 46.831 | 63.556 | 1.00 | 48.06 |
| ATOM | 5033 | O | HOH | W | 125 | -17.843 | 39.367 | 36.020 | 1.00 | 35.80 |
| ATOM | 5034 | O | HOH | W | 126 | 2.218   | 57.766 | 62.253 | 1.00 | 44.6  |
| ATOM | 5035 | O | HOH | W | 127 | 10.736  | 62.766 | 64.366 | 1.00 | 55.84 |
| ATOM | 5036 | O | HOH | W | 128 | 0.884   | 35.562 | 63.963 | 1.00 | 44.14 |
| ATOM | 5037 | O | HOH | W | 129 | 19.165  | 59.557 | 60.644 | 1.00 | 47.82 |
| ATOM | 5038 | O | HOH | W | 130 | 1.546   | 27.875 | 68.443 | 1.00 | 39.69 |
| ATOM | 5039 | O | HOH | W | 131 | 5.497   | 26.285 | 76.668 | 1.00 | 44.47 |
| ATOM | 5040 | O | HOH | W | 132 | 14.505  | 36.538 | 88.996 | 1.00 | 40.00 |
| ATOM | 5041 | O | HOH | W | 133 | 8.534   | 28.713 | 88.519 | 1.00 | 46.55 |
| ATOM | 5042 | O | HOH | W | 134 | 6.125   | 45.267 | 77.959 | 1.00 | 45.57 |
| ATOM | 5043 | O | HOH | W | 135 | 26.016  | 18.543 | 78.878 | 1.00 | 51.65 |
| ATOM | 5044 | O | HOH | W | 136 | 33.880  | 23.025 | 70.739 | 1.00 | 46.95 |
| ATOM | 5045 | O | HOH | W | 137 | 19.230  | 26.073 | 49.998 | 1.00 | 51.97 |
| ATOM | 5046 | O | HOH | W | 138 | 41.563  | 41.085 | 77.326 | 1.00 | 43.14 |
| ATOM | 5047 | O | HOH | W | 139 | 39.187  | 63.067 | 75.380 | 1.00 | 56.52 |
| ATOM | 5048 | O | HOH | W | 140 | 26.878  | 54.491 | 67.203 | 1.00 | 42.14 |
| ATOM | 5049 | O | HOH | W | 141 | 22.988  | 62.189 | 74.174 | 1.00 | 48.31 |
| ATOM | 5050 | O | HOH | W | 142 | 25.190  | 62.803 | 71.067 | 1.00 | 67.16 |
| ATOM | 5051 | O | HOH | W | 143 | 18.598  | 45.126 | 81.949 | 1.00 | 53.80 |
| ATOM | 5052 | O | HOH | W | 144 | 19.782  | 53.129 | 90.556 | 1.00 | 48.73 |
| ATOM | 5053 | O | HOH | W | 145 | 21.735  | 48.367 | 86.454 | 1.00 | 40.39 |
| ATOM | 5054 | O | HOH | W | 146 | 25.707  | 57.012 | 93.476 | 1.00 | 53.61 |
| ATOM | 5055 | O | HOH | W | 147 | 22.832  | 62.085 | 93.149 | 1.00 | 46.02 |
| ATOM | 5056 | O | HOH | W | 148 | 25.725  | 67.203 | 89.990 | 1.00 | 75.23 |
| ATOM | 5057 | O | HOH | W | 149 | 10.773  | 53.653 | 85.697 | 1.00 | 50.65 |
| ATOM | 5058 | O | HOH | W | 150 | 4.221   | 58.449 | 86.608 | 1.00 | 49.23 |
| ATOM | 5059 | O | HOH | W | 151 | 7.790   | 72.096 | 84.410 | 1.00 | 51.10 |
| ATOM | 5060 | O | HOH | W | 152 | 2.387   | 58.282 | 67.835 | 1.00 | 33.29 |
| ATOM | 5061 | O | HOH | W | 153 | 0.921   | 49.551 | 69.095 | 1.00 | 59.60 |
| ATOM | 5062 | O | HOH | W | 154 | 8.722   | 45.171 | 71.561 | 1.00 | 46.56 |
| ATOM | 5063 | O | HOH | W | 155 | 6.422   | 47.947 | 81.081 | 1.00 | 57.56 |
| ATOM | 5064 | O | HOH | W | 156 | 15.936  | 56.908 | 55.129 | 1.00 | 43.33 |
| ATOM | 5065 | O | HOH | W | 157 | 3.032   | 19.635 | 62.453 | 1.00 | 80.38 |
| ATOM | 5066 | O | HOH | W | 158 | -4.228  | 58.058 | 47.057 | 1.00 | 39.66 |
| ATOM | 5067 | O | HOH | W | 1   |         |        |        |      |       |



5012240:022500

|      |      |   |           |         |        |        |      |       |
|------|------|---|-----------|---------|--------|--------|------|-------|
| ATOM | 5083 | O | HOH W 175 | 18.301  | 47.296 | 43.793 | 1.00 | 45.84 |
| ATOM | 5084 | O | HOH W 176 | 11.717  | 61.868 | 52.648 | 1.00 | 34.93 |
| ATOM | 5085 | O | HOH W 177 | 29.516  | 23.822 | 76.838 | 1.00 | 51.50 |
| ATOM | 5086 | O | HOH W 178 | 39.940  | 60.509 | 78.535 | 1.00 | 46.33 |
| ATOM | 5087 | O | HOH W 179 | -1.803  | 44.974 | 37.278 | 1.00 | 52.56 |
| ATOM | 5088 | O | HOH W 180 | 7.343   | 47.305 | 65.468 | 1.00 | 47.27 |
| ATOM | 5089 | O | HOH W 181 | 17.912  | 15.338 | 81.793 | 1.00 | 50.08 |
| ATOM | 5090 | O | HOH W 182 | -4.631  | 55.917 | 82.183 | 1.00 | 65.36 |
| ATOM | 5091 | O | HOH W 183 | 32.973  | 42.656 | 86.667 | 1.00 | 43.97 |
| ATOM | 5092 | O | HOH W 184 | -1.834  | 36.784 | 71.040 | 1.00 | 45.10 |
| ATOM | 5093 | O | HOH W 185 | -4.519  | 34.633 | 71.838 | 1.00 | 43.99 |
| ATOM | 5094 | O | HOH W 186 | 4.518   | 68.554 | 71.661 | 1.00 | 46.99 |
| ATOM | 5095 | O | HOH W 187 | 2.774   | 37.503 | 61.490 | 1.00 | 45.81 |
| ATOM | 5096 | O | HOH W 188 | 31.770  | 43.526 | 51.410 | 1.00 | 58.02 |
| ATOM | 5097 | O | HOH W 189 | 5.471   | 43.861 | 38.891 | 1.00 | 49.43 |
| ATOM | 5098 | O | HOH W 190 | 11.934  | 58.219 | 70.811 | 1.00 | 49.96 |
| ATOM | 5099 | O | HOH W 191 | 33.112  | 26.203 | 70.484 | 1.00 | 60.03 |
| ATOM | 5100 | O | HOH W 192 | 30.914  | 43.017 | 70.613 | 1.00 | 73.23 |
| ATOM | 5101 | O | HOH W 193 | 0.400   | 39.300 | 39.714 | 1.00 | 65.37 |
| ATOM | 5102 | O | HOH W 194 | 48.247  | 56.159 | 86.370 | 1.00 | 60.09 |
| ATOM | 5103 | O | HOH W 195 | 12.359  | 59.992 | 62.698 | 1.00 | 53.57 |
| ATOM | 5104 | O | HOH W 196 | 11.149  | 17.504 | 78.264 | 1.00 | 54.43 |
| ATOM | 5105 | O | HOH W 197 | -4.284  | 31.953 | 60.991 | 1.00 | 47.12 |
| ATOM | 5106 | O | HOH W 198 | 29.888  | 35.624 | 82.772 | 1.00 | 52.16 |
| ATOM | 5107 | O | HOH W 199 | 14.388  | 39.115 | 89.656 | 1.00 | 47.93 |
| ATOM | 5108 | O | HOH W 200 | -8.529  | 51.475 | 47.745 | 1.00 | 61.00 |
| ATOM | 5109 | O | HOH W 201 | -15.572 | 53.338 | 52.008 | 1.00 | 72.42 |
| ATOM | 5110 | O | HOH W 202 | 24.319  | 38.590 | 87.128 | 1.00 | 50.03 |
| ATOM | 5111 | O | HOH W 203 | 25.366  | 70.670 | 82.839 | 1.00 | 49.01 |
| ATOM | 5112 | O | HOH W 204 | 18.531  | 27.749 | 86.236 | 1.00 | 48.64 |
| ATOM | 5113 | O | HOH W 205 | 21.694  | 20.030 | 81.796 | 1.00 | 49.04 |
| ATOM | 5114 | O | HOH W 206 | 23.953  | 47.993 | 67.580 | 1.00 | 40.39 |
| ATOM | 5115 | O | HOH W 207 | 22.012  | 40.217 | 90.228 | 1.00 | 42.29 |
| ATOM | 5116 | O | HOH W 208 | 16.197  | 45.094 | 43.427 | 1.00 | 48.00 |
| ATOM | 5117 | O | HOH W 209 | 21.019  | 68.985 | 84.382 | 1.00 | 56.50 |
| ATOM | 5118 | O | HOH W 210 | -7.134  | 33.015 | 71.591 | 1.00 | 56.31 |
| ATOM | 5119 | O | HOH W 211 | 40.843  | 44.050 | 89.284 | 1.00 | 43.07 |
| ATOM | 5120 | O | HOH W 212 | 20.374  | 14.856 | 56.642 | 1.00 | 50.07 |
| ATOM | 5121 | O | HOH W 213 | 12.723  | 46.277 | 73.748 | 1.00 | 59.15 |
| ATOM | 5122 | O | HOH W 214 | 8.956   | 43.704 | 58.706 | 1.00 | 45.56 |
| ATOM | 5123 | O | HOH W 215 | -2.433  | 36.012 | 80.232 | 1.00 | 54.12 |
| ATOM | 5124 | O | HOH W 216 | 5.257   | 25.271 | 55.914 | 1.00 | 53.23 |
| ATOM | 5125 | O | HOH W 217 | 13.354  | 64.403 | 53.862 | 1.00 | 47.27 |
| ATOM | 5126 | O | HOH W 218 | 30.477  | 42.517 | 67.472 | 1.00 | 48.17 |
| ATOM | 5127 | O | HOH W 219 | 14.139  | 47.479 | 76.123 | 1.00 | 79.04 |
| ATOM | 5128 | O | HOH W 220 | 0.829   | 29.563 | 50.769 | 1.00 | 48.10 |
| ATOM | 5129 | O | HOH W 221 | 32.979  | 51.667 | 96.624 | 1.00 | 51.30 |
| ATOM | 5130 | O | HOH W 222 | 14.677  | 45.948 | 71.756 | 1.00 | 52.31 |
| ATOM | 5131 | O | HOH W 223 | 33.890  | 24.505 | 58.094 | 1.00 | 43.65 |
| ATOM | 5132 | O | HOH W 224 | 17.853  | 9.519  | 65.560 | 1.00 | 55.94 |
| ATOM | 5133 | O | HOH W 225 | 37.794  | 31.473 | 62.305 | 1.00 | 50.38 |
| ATOM | 5134 | O | HOH W 226 | 29.206  | 50.335 | 62.673 | 1.00 | 45.43 |
| ATOM | 5135 | O | HOH W 227 | 4.932   | 48.808 | 63.354 | 1.00 | 42.45 |
| ATOM | 5136 | O | HOH W 228 | 18.933  | 59.070 | 55.899 | 1.00 | 50.29 |
| ATOM | 5137 | O | HOH W 229 | 13.849  | 18.833 | 83.641 | 1.00 | 55.89 |
| ATOM | 5138 | O | HOH W 230 | 25.919  | 46.022 | 68.076 | 1.00 | 35.63 |
| ATOM | 5139 | O | HOH W 231 | 27.565  | 65.098 | 75.153 | 1.00 | 73.11 |
| ATOM | 5140 | O | HOH W 232 | 27.128  | 39.012 | 68.497 | 1.00 | 40.77 |



001210 000000

|      |      |   |           |         |        |        |      |       |
|------|------|---|-----------|---------|--------|--------|------|-------|
| ATOM | 5141 | O | HOH W 233 | 40.706  | 52.468 | 74.641 | 1.00 | 51.60 |
| ATOM | 5142 | O | HOH W 234 | 21.689  | 65.312 | 58.080 | 1.00 | 66.72 |
| ATOM | 5143 | O | HOH W 235 | 9.121   | 17.615 | 59.271 | 1.00 | 51.98 |
| ATOM | 5144 | O | HOH W 236 | 17.931  | 36.565 | 88.091 | 1.00 | 54.77 |
| ATOM | 5145 | O | HOH W 237 | 33.843  | 36.707 | 52.576 | 1.00 | 61.60 |
| ATOM | 5146 | O | HOH W 238 | -3.693  | 50.074 | 63.986 | 1.00 | 43.64 |
| ATOM | 5147 | O | HOH W 239 | 44.272  | 44.279 | 81.461 | 1.00 | 69.21 |
| ATOM | 5148 | O | HOH W 240 | 2.092   | 28.868 | 52.894 | 1.00 | 54.01 |
| ATOM | 5149 | O | HOH W 241 | 8.309   | 33.518 | 71.442 | 1.00 | 68.05 |
| ATOM | 5150 | O | HOH W 242 | 1.051   | 31.947 | 69.204 | 1.00 | 52.88 |
| ATOM | 5151 | O | HOH W 243 | 44.255  | 51.162 | 96.650 | 1.00 | 20.00 |
| ATOM | 5152 | O | HOH W 244 | 16.173  | 45.408 | 46.636 | 1.00 | 20.00 |
| ATOM | 5153 | O | HOH W 245 | 41.130  | 50.734 | 97.991 | 1.00 | 20.00 |
| ATOM | 5154 | O | HOH W 246 | 36.912  | 36.263 | 75.911 | 1.00 | 20.00 |
| ATOM | 5155 | O | HOH W 247 | -17.107 | 27.146 | 54.728 | 1.00 | 20.00 |
| ATOM | 5156 | O | HOH W 248 | 24.078  | 46.307 | 79.123 | 1.00 | 20.00 |
| ATOM | 5157 | O | HOH W 249 | -12.250 | 47.964 | 61.593 | 1.00 | 20.00 |
| ATOM | 5158 | O | HOH W 250 | 35.804  | 51.343 | 51.682 | 1.00 | 20.00 |
| ATOM | 5159 | O | HOH W 251 | 25.537  | 59.940 | 69.750 | 1.00 | 20.00 |
| ATOM | 5160 | O | HOH W 252 | 0.539   | 55.427 | 62.088 | 1.00 | 20.00 |
| END  |      |   |           |         |        |        |      |       |



Table 11: Structure coordinates of LTA<sub>4</sub> hydrolase-hydroxamic acid complex

| CRYST | 67.770 | 132.470 | 83.700    | 90.00 | 90.00  | 90.00  | P21212 |            |
|-------|--------|---------|-----------|-------|--------|--------|--------|------------|
|       | Atom   | res.    | Chain No. | x     | y      | z      | occ    | B-factor   |
| ATOM  | 1      | N       | PRO A     | 1     | -2.215 | 16.942 | 65.912 | 1.00 98.67 |
| ATOM  | 2      | CA      | PRO A     | 1     | -2.492 | 18.109 | 66.739 | 1.00 96.57 |
| ATOM  | 3      | C       | PRO A     | 1     | -1.985 | 19.345 | 66.046 | 1.00 90.92 |
| ATOM  | 4      | O       | PRO A     | 1     | -0.791 | 19.459 | 65.732 | 1.00 87.94 |
| ATOM  | 5      | CB      | PRO A     | 1     | -1.747 | 17.907 | 68.073 | 1.00 98.18 |
| ATOM  | 6      | CG      | PRO A     | 1     | -1.000 | 16.573 | 67.973 | 1.00100.00 |
| ATOM  | 7      | CD      | PRO A     | 1     | -1.249 | 16.011 | 66.573 | 1.00 97.96 |
| ATOM  | 8      | N       | GLU A     | 2     | -2.895 | 20.262 | 65.790 | 1.00 83.08 |
| ATOM  | 9      | CA      | GLU A     | 2     | -2.492 | 21.448 | 65.116 | 1.00 81.25 |
| ATOM  | 10     | C       | GLU A     | 2     | -1.948 | 22.471 | 66.074 | 1.00 80.21 |
| ATOM  | 11     | O       | GLU A     | 2     | -2.444 | 22.625 | 67.189 | 1.00 80.90 |
| ATOM  | 12     | CB      | GLU A     | 2     | -3.549 | 22.038 | 64.168 | 1.00 82.10 |
| ATOM  | 13     | CG      | GLU A     | 2     | -2.895 | 22.838 | 63.023 | 1.00 92.94 |
| ATOM  | 14     | CD      | GLU A     | 2     | -1.451 | 22.466 | 62.778 | 1.00 95.77 |
| ATOM  | 15     | OE1     | GLU A     | 2     | -0.520 | 23.237 | 62.917 | 1.00 94.64 |
| ATOM  | 16     | OE2     | GLU A     | 2     | -1.307 | 21.231 | 62.383 | 1.00 74.00 |
| ATOM  | 17     | N       | ILE A     | 3     | -0.898 | 23.141 | 65.624 | 1.00 69.91 |
| ATOM  | 18     | CA      | ILE A     | 3     | -0.300 | 24.192 | 66.393 | 1.00 66.19 |
| ATOM  | 19     | C       | ILE A     | 3     | -1.124 | 25.431 | 66.042 | 1.00 60.35 |
| ATOM  | 20     | O       | ILE A     | 3     | -1.438 | 25.713 | 64.866 | 1.00 60.57 |
| ATOM  | 21     | CB      | ILE A     | 3     | 1.215  | 24.316 | 66.167 | 1.00 69.46 |
| ATOM  | 22     | CG1     | ILE A     | 3     | 1.919  | 23.117 | 66.809 | 1.00 69.22 |
| ATOM  | 23     | CG2     | ILE A     | 3     | 1.772  | 25.604 | 66.769 | 1.00 70.57 |
| ATOM  | 24     | CD1     | ILE A     | 3     | 2.674  | 23.468 | 68.090 | 1.00 67.16 |
| ATOM  | 25     | N       | VAL A     | 4     | -1.546 | 26.135 | 67.071 | 1.00 47.12 |
| ATOM  | 26     | CA      | VAL A     | 4     | -2.372 | 27.296 | 66.856 | 1.00 43.66 |
| ATOM  | 27     | C       | VAL A     | 4     | -1.621 | 28.601 | 66.943 | 1.00 36.61 |
| ATOM  | 28     | O       | VAL A     | 4     | -0.804 | 28.799 | 67.843 | 1.00 33.97 |
| ATOM  | 29     | CB      | VAL A     | 4     | -3.580 | 27.282 | 67.811 | 1.00 46.37 |
| ATOM  | 30     | CG1     | VAL A     | 4     | -4.296 | 28.636 | 67.855 | 1.00 44.31 |
| ATOM  | 31     | CG2     | VAL A     | 4     | -4.552 | 26.203 | 67.353 | 1.00 45.89 |
| ATOM  | 32     | N       | ASP A     | 5     | -1.920 | 29.496 | 65.997 | 1.00 25.42 |
| ATOM  | 33     | CA      | ASP A     | 5     | -1.311 | 30.793 | 66.050 | 1.00 22.70 |
| ATOM  | 34     | C       | ASP A     | 5     | -2.262 | 31.630 | 66.874 | 1.00 26.31 |
| ATOM  | 35     | O       | ASP A     | 5     | -3.285 | 32.069 | 66.397 | 1.00 25.00 |
| ATOM  | 36     | CB      | ASP A     | 5     | -1.083 | 31.454 | 64.687 | 1.00 23.91 |
| ATOM  | 37     | CG      | ASP A     | 5     | -0.248 | 32.685 | 64.868 | 1.00 28.48 |
| ATOM  | 38     | OD1     | ASP A     | 5     | -0.199 | 33.272 | 65.935 | 1.00 27.12 |
| ATOM  | 39     | OD2     | ASP A     | 5     | 0.383  | 33.068 | 63.776 | 1.00 23.01 |
| ATOM  | 40     | N       | THR A     | 6     | -1.942 | 31.792 | 68.144 | 1.00 25.96 |
| ATOM  | 41     | CA      | THR A     | 6     | -2.799 | 32.525 | 69.029 | 1.00 23.74 |
| ATOM  | 42     | C       | THR A     | 6     | -2.689 | 34.005 | 68.859 | 1.00 27.92 |
| ATOM  | 43     | O       | THR A     | 6     | -3.169 | 34.763 | 69.701 | 1.00 31.80 |
| ATOM  | 44     | CB      | THR A     | 6     | -2.629 | 32.111 | 70.483 | 1.00 25.94 |
| ATOM  | 45     | OG1     | THR A     | 6     | -1.315 | 32.422 | 70.891 | 1.00 40.88 |
| ATOM  | 46     | CG2     | THR A     | 6     | -2.867 | 30.609 | 70.627 | 1.00 29.05 |
| ATOM  | 47     | N       | CYS A     | 7     | -2.068 | 34.442 | 67.779 | 1.00 23.72 |
| ATOM  | 48     | CA      | CYS A     | 7     | -1.967 | 35.893 | 67.566 | 1.00 24.38 |
| ATOM  | 49     | C       | CYS A     | 7     | -2.737 | 36.321 | 66.325 | 1.00 28.42 |
| ATOM  | 50     | O       | CYS A     | 7     | -2.766 | 37.475 | 65.965 | 1.00 27.59 |
| ATOM  | 51     | CB      | CYS A     | 7     | -0.516 | 36.435 | 67.449 | 1.00 23.86 |
| ATOM  | 52     | SG      | CYS A     | 7     | 0.510  | 36.080 | 68.886 | 1.00 29.33 |



|      |     |     |     |   |    |         |        |        |      |       |
|------|-----|-----|-----|---|----|---------|--------|--------|------|-------|
| ATOM | 53  | N   | SER | A | 8  | -3.324  | 35.370 | 65.638 | 1.00 | 27.23 |
| ATOM | 54  | CA  | SER | A | 8  | -4.020  | 35.686 | 64.419 | 1.00 | 25.64 |
| ATOM | 55  | C   | SER | A | 8  | -5.479  | 35.340 | 64.538 | 1.00 | 25.31 |
| ATOM | 56  | O   | SER | A | 8  | -5.867  | 34.421 | 65.273 | 1.00 | 22.83 |
| ATOM | 57  | CB  | SER | A | 8  | -3.368  | 34.908 | 63.278 | 1.00 | 26.35 |
| ATOM | 58  | OG  | SER | A | 8  | -4.090  | 35.105 | 62.093 | 1.00 | 29.02 |
| ATOM | 59  | N   | LEU | A | 9  | -6.298  | 36.071 | 63.799 | 1.00 | 20.95 |
| ATOM | 60  | CA  | LEU | A | 9  | -7.720  | 35.750 | 63.869 | 1.00 | 20.81 |
| ATOM | 61  | C   | LEU | A | 9  | -8.188  | 35.158 | 62.554 | 1.00 | 24.77 |
| ATOM | 62  | O   | LEU | A | 9  | -9.364  | 34.872 | 62.381 | 1.00 | 28.22 |
| ATOM | 63  | CB  | LEU | A | 9  | -8.573  | 36.991 | 64.170 | 1.00 | 20.29 |
| ATOM | 64  | CG  | LEU | A | 9  | -8.171  | 37.744 | 65.434 | 1.00 | 21.06 |
| ATOM | 65  | CD1 | LEU | A | 9  | -8.875  | 39.088 | 65.438 | 1.00 | 22.40 |
| ATOM | 66  | CD2 | LEU | A | 9  | -8.576  | 36.926 | 66.656 | 1.00 | 15.77 |
| ATOM | 67  | N   | ALA | A | 10 | -7.240  | 35.040 | 61.630 | 1.00 | 22.60 |
| ATOM | 68  | CA  | ALA | A | 10 | -7.461  | 34.528 | 60.294 | 1.00 | 17.85 |
| ATOM | 69  | C   | ALA | A | 10 | -7.633  | 33.039 | 60.254 | 1.00 | 23.94 |
| ATOM | 70  | O   | ALA | A | 10 | -7.281  | 32.298 | 61.178 | 1.00 | 22.85 |
| ATOM | 71  | CB  | ALA | A | 10 | -6.291  | 34.891 | 59.397 | 1.00 | 15.48 |
| ATOM | 72  | N   | SER | A | 11 | -8.170  | 32.590 | 59.129 | 1.00 | 25.50 |
| ATOM | 73  | CA  | SER | A | 11 | -8.306  | 31.156 | 58.921 | 1.00 | 27.59 |
| ATOM | 74  | C   | SER | A | 11 | -6.887  | 30.575 | 58.992 | 1.00 | 25.13 |
| ATOM | 75  | O   | SER | A | 11 | -5.938  | 31.112 | 58.437 | 1.00 | 26.43 |
| ATOM | 76  | CB  | SER | A | 11 | -8.917  | 30.833 | 57.544 | 1.00 | 29.01 |
| ATOM | 77  | OG  | SER | A | 11 | -10.241 | 31.338 | 57.445 | 1.00 | 28.50 |
| ATOM | 78  | N   | PRO | A | 12 | -6.740  | 29.460 | 59.662 | 1.00 | 23.36 |
| ATOM | 79  | CA  | PRO | A | 12 | -5.445  | 28.827 | 59.798 | 1.00 | 20.96 |
| ATOM | 80  | C   | PRO | A | 12 | -4.949  | 28.121 | 58.533 | 1.00 | 34.02 |
| ATOM | 81  | O   | PRO | A | 12 | -5.743  | 27.764 | 57.646 | 1.00 | 34.95 |
| ATOM | 82  | CB  | PRO | A | 12 | -5.590  | 27.834 | 60.952 | 1.00 | 22.26 |
| ATOM | 83  | CG  | PRO | A | 12 | -7.080  | 27.652 | 61.201 | 1.00 | 29.49 |
| ATOM | 84  | CD  | PRO | A | 12 | -7.769  | 28.845 | 60.542 | 1.00 | 25.95 |
| ATOM | 85  | N   | ALA | A | 13 | -3.615  | 27.927 | 58.479 | 1.00 | 29.46 |
| ATOM | 86  | CA  | ALA | A | 13 | -2.922  | 27.276 | 57.385 | 1.00 | 25.81 |
| ATOM | 87  | C   | ALA | A | 13 | -3.531  | 25.912 | 57.109 | 1.00 | 27.87 |
| ATOM | 88  | O   | ALA | A | 13 | -3.320  | 25.321 | 56.072 | 1.00 | 30.10 |
| ATOM | 89  | CB  | ALA | A | 13 | -1.458  | 27.115 | 57.746 | 1.00 | 25.60 |
| ATOM | 90  | N   | SER | A | 14 | -4.288  | 25.389 | 58.038 | 1.00 | 20.61 |
| ATOM | 91  | CA  | SER | A | 14 | -4.876  | 24.090 | 57.814 | 1.00 | 24.37 |
| ATOM | 92  | C   | SER | A | 14 | -6.230  | 24.183 | 57.108 | 1.00 | 32.80 |
| ATOM | 93  | O   | SER | A | 14 | -6.831  | 23.183 | 56.733 | 1.00 | 35.15 |
| ATOM | 94  | CB  | SER | A | 14 | -5.031  | 23.366 | 59.137 | 1.00 | 29.06 |
| ATOM | 95  | OG  | SER | A | 14 | -5.775  | 24.180 | 60.037 | 1.00 | 31.14 |
| ATOM | 96  | N   | VAL | A | 15 | -6.721  | 25.392 | 56.944 | 1.00 | 24.99 |
| ATOM | 97  | CA  | VAL | A | 15 | -7.984  | 25.582 | 56.278 | 1.00 | 25.26 |
| ATOM | 98  | C   | VAL | A | 15 | -7.774  | 26.148 | 54.865 | 1.00 | 27.71 |
| ATOM | 99  | O   | VAL | A | 15 | -8.348  | 25.688 | 53.886 | 1.00 | 27.54 |
| ATOM | 100 | CB  | VAL | A | 15 | -8.876  | 26.466 | 57.127 | 1.00 | 29.72 |
| ATOM | 101 | CG1 | VAL | A | 15 | -9.999  | 27.045 | 56.271 | 1.00 | 30.81 |
| ATOM | 102 | CG2 | VAL | A | 15 | -9.411  | 25.656 | 58.298 | 1.00 | 27.89 |
| ATOM | 103 | N   | CYS | A | 16 | -6.921  | 27.144 | 54.764 | 1.00 | 20.14 |
| ATOM | 104 | CA  | CYS | A | 16 | -6.594  | 27.769 | 53.503 | 1.00 | 24.17 |
| ATOM | 105 | C   | CYS | A | 16 | -5.265  | 28.490 | 53.629 | 1.00 | 26.96 |
| ATOM | 106 | O   | CYS | A | 16 | -4.834  | 28.793 | 54.744 | 1.00 | 28.25 |
| ATOM | 107 | CB  | CYS | A | 16 | -7.703  | 28.694 | 52.944 | 1.00 | 28.08 |
| ATOM | 108 | SG  | CYS | A | 16 | -7.881  | 30.231 | 53.880 | 1.00 | 34.58 |
| ATOM | 109 | N   | ARG | A | 17 | -4.622  | 28.749 | 52.496 | 1.00 | 20.39 |
| ATOM | 110 | CA  | ARG | A | 17 | -3.344  | 29.409 | 52.520 | 1.00 | 22.15 |



|      |     |     |     |   |    |        |        |        |      |       |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|
| ATOM | 111 | C   | ARG | A | 17 | -3.186 | 30.347 | 51.365 | 1.00 | 26.96 |
| ATOM | 112 | O   | ARG | A | 17 | -3.415 | 30.002 | 50.202 | 1.00 | 23.44 |
| ATOM | 113 | CB  | ARG | A | 17 | -2.147 | 28.451 | 52.443 | 1.00 | 26.39 |
| ATOM | 114 | CG  | ARG | A | 17 | -2.231 | 27.181 | 53.264 | 1.00 | 24.30 |
| ATOM | 115 | CD  | ARG | A | 17 | -1.416 | 26.086 | 52.599 | 1.00 | 28.56 |
| ATOM | 116 | NE  | ARG | A | 17 | -0.772 | 25.134 | 53.510 | 1.00 | 51.45 |
| ATOM | 117 | CZ  | ARG | A | 17 | -1.392 | 24.225 | 54.263 | 1.00 | 69.75 |
| ATOM | 118 | NH1 | ARG | A | 17 | -2.693 | 24.086 | 54.287 | 1.00 | 72.82 |
| ATOM | 119 | NH2 | ARG | A | 17 | -0.694 | 23.418 | 55.032 | 1.00 | 48.88 |
| ATOM | 120 | N   | THR | A | 18 | -2.723 | 31.532 | 51.700 | 1.00 | 21.89 |
| ATOM | 121 | CA  | THR | A | 18 | -2.478 | 32.539 | 50.713 | 1.00 | 20.46 |
| ATOM | 122 | C   | THR | A | 18 | -1.200 | 32.197 | 50.007 | 1.00 | 27.00 |
| ATOM | 123 | O   | THR | A | 18 | -0.207 | 31.923 | 50.662 | 1.00 | 26.28 |
| ATOM | 124 | CB  | THR | A | 18 | -2.370 | 33.949 | 51.337 | 1.00 | 21.64 |
| ATOM | 125 | OG1 | THR | A | 18 | -3.539 | 34.262 | 52.076 | 1.00 | 25.03 |
| ATOM | 126 | CG2 | THR | A | 18 | -2.164 | 34.944 | 50.211 | 1.00 | 21.73 |
| ATOM | 127 | N   | LYS | A | 19 | -1.235 | 32.203 | 48.677 | 1.00 | 22.54 |
| ATOM | 128 | CA  | LYS | A | 19 | -0.091 | 31.871 | 47.864 | 1.00 | 21.16 |
| ATOM | 129 | C   | LYS | A | 19 | 0.538  | 33.063 | 47.238 | 1.00 | 23.51 |
| ATOM | 130 | O   | LYS | A | 19 | 1.732  | 33.098 | 46.968 | 1.00 | 23.00 |
| ATOM | 131 | CB  | LYS | A | 19 | -0.557 | 30.976 | 46.740 | 1.00 | 24.60 |
| ATOM | 132 | CG  | LYS | A | 19 | -1.311 | 29.775 | 47.257 | 1.00 | 34.24 |
| ATOM | 133 | CD  | LYS | A | 19 | -0.944 | 29.419 | 48.688 | 1.00 | 65.32 |
| ATOM | 134 | CE  | LYS | A | 19 | 0.230  | 28.442 | 48.793 | 1.00 | 75.40 |
| ATOM | 135 | NZ  | LYS | A | 19 | 1.183  | 28.796 | 49.864 | 1.00 | 66.99 |
| ATOM | 136 | N   | HIS | A | 20 | -0.280 | 34.053 | 46.967 | 1.00 | 22.30 |
| ATOM | 137 | CA  | HIS | A | 20 | 0.201  | 35.250 | 46.309 | 1.00 | 20.94 |
| ATOM | 138 | C   | HIS | A | 20 | -0.588 | 36.484 | 46.673 | 1.00 | 23.90 |
| ATOM | 139 | O   | HIS | A | 20 | -1.779 | 36.414 | 47.022 | 1.00 | 23.31 |
| ATOM | 140 | CB  | HIS | A | 20 | 0.054  | 35.095 | 44.801 | 1.00 | 19.15 |
| ATOM | 141 | CG  | HIS | A | 20 | 0.888  | 36.085 | 44.129 | 1.00 | 20.96 |
| ATOM | 142 | ND1 | HIS | A | 20 | 2.258  | 36.003 | 44.163 | 1.00 | 22.60 |
| ATOM | 143 | CD2 | HIS | A | 20 | 0.538  | 37.198 | 43.437 | 1.00 | 24.10 |
| ATOM | 144 | CE1 | HIS | A | 20 | 2.725  | 37.040 | 43.496 | 1.00 | 23.71 |
| ATOM | 145 | NE2 | HIS | A | 20 | 1.708  | 37.784 | 43.025 | 1.00 | 24.51 |
| ATOM | 146 | N   | LEU | A | 21 | 0.105  | 37.600 | 46.594 | 1.00 | 26.18 |
| ATOM | 147 | CA  | LEU | A | 21 | -0.484 | 38.893 | 46.871 | 1.00 | 27.24 |
| ATOM | 148 | C   | LEU | A | 21 | -0.104 | 39.856 | 45.805 | 1.00 | 27.01 |
| ATOM | 149 | O   | LEU | A | 21 | 1.076  | 40.014 | 45.522 | 1.00 | 27.97 |
| ATOM | 150 | CB  | LEU | A | 21 | -0.064 | 39.501 | 48.215 | 1.00 | 28.80 |
| ATOM | 151 | CG  | LEU | A | 21 | -0.335 | 41.006 | 48.296 | 1.00 | 34.13 |
| ATOM | 152 | CD1 | LEU | A | 21 | -1.834 | 41.309 | 48.440 | 1.00 | 36.26 |
| ATOM | 153 | CD2 | LEU | A | 21 | 0.393  | 41.578 | 49.504 | 1.00 | 36.24 |
| ATOM | 154 | N   | HIS | A | 22 | -1.110 | 40.475 | 45.203 | 1.00 | 28.25 |
| ATOM | 155 | CA  | HIS | A | 22 | -0.852 | 41.482 | 44.186 | 1.00 | 30.03 |
| ATOM | 156 | C   | HIS | A | 22 | -1.272 | 42.800 | 44.795 | 1.00 | 31.36 |
| ATOM | 157 | O   | HIS | A | 22 | -2.435 | 42.993 | 45.127 | 1.00 | 30.57 |
| ATOM | 158 | CB  | HIS | A | 22 | -1.560 | 41.291 | 42.844 | 1.00 | 31.66 |
| ATOM | 159 | CG  | HIS | A | 22 | -1.060 | 42.347 | 41.913 | 1.00 | 34.36 |
| ATOM | 160 | ND1 | HIS | A | 22 | -1.913 | 43.134 | 41.187 | 1.00 | 37.39 |
| ATOM | 161 | CD2 | HIS | A | 22 | 0.208  | 42.734 | 41.635 | 1.00 | 37.45 |
| ATOM | 162 | CE1 | HIS | A | 22 | -1.155 | 43.968 | 40.481 | 1.00 | 38.02 |
| ATOM | 163 | NE2 | HIS | A | 22 | 0.132  | 43.757 | 40.730 | 1.00 | 37.95 |
| ATOM | 164 | N   | LEU | A | 23 | -0.315 | 43.668 | 45.000 | 1.00 | 31.07 |
| ATOM | 165 | CA  | LEU | A | 23 | -0.593 | 44.939 | 45.637 | 1.00 | 31.63 |
| ATOM | 166 | C   | LEU | A | 23 | -0.469 | 46.144 | 44.705 | 1.00 | 32.72 |
| ATOM | 167 | O   | LEU | A | 23 | 0.563  | 46.431 | 44.093 | 1.00 | 34.74 |
| ATOM | 168 | CB  | LEU | A | 23 | 0.299  | 45.093 | 46.894 | 1.00 | 31.20 |



|      |     |     |     |   |    |        |        |        |      |        |
|------|-----|-----|-----|---|----|--------|--------|--------|------|--------|
| ATOM | 169 | CG  | LEU | A | 23 | -0.320 | 45.795 | 48.126 | 1.00 | 34.26  |
| ATOM | 170 | CD1 | LEU | A | 23 | 0.543  | 46.966 | 48.510 | 1.00 | 32.64  |
| ATOM | 171 | CD2 | LEU | A | 23 | -1.759 | 46.263 | 47.957 | 1.00 | 34.32  |
| ATOM | 172 | N   | ARG | A | 24 | -1.576 | 46.840 | 44.623 | 1.00 | 28.33  |
| ATOM | 173 | CA  | ARG | A | 24 | -1.681 | 48.040 | 43.837 | 1.00 | 30.28  |
| ATOM | 174 | C   | ARG | A | 24 | -2.162 | 49.119 | 44.794 | 1.00 | 35.16  |
| ATOM | 175 | O   | ARG | A | 24 | -3.251 | 49.005 | 45.349 | 1.00 | 35.74  |
| ATOM | 176 | CB  | ARG | A | 24 | -2.651 | 47.860 | 42.689 | 1.00 | 32.69  |
| ATOM | 177 | CG  | ARG | A | 24 | -1.962 | 47.363 | 41.423 | 1.00 | 55.58  |
| ATOM | 178 | CD  | ARG | A | 24 | -2.732 | 47.698 | 40.144 | 1.00 | 67.44  |
| ATOM | 179 | NE  | ARG | A | 24 | -3.993 | 46.971 | 40.030 | 1.00 | 64.57  |
| ATOM | 180 | CZ  | ARG | A | 24 | -5.150 | 47.440 | 40.498 | 1.00 | 97.41  |
| ATOM | 181 | NH1 | ARG | A | 24 | -5.246 | 48.624 | 41.108 | 1.00 | 81.55  |
| ATOM | 182 | NH2 | ARG | A | 24 | -6.249 | 46.713 | 40.344 | 1.00 | 100.00 |
| ATOM | 183 | N   | CYS | A | 25 | -1.320 | 50.126 | 45.045 | 1.00 | 36.40  |
| ATOM | 184 | CA  | CYS | A | 25 | -1.696 | 51.181 | 45.998 | 1.00 | 36.70  |
| ATOM | 185 | C   | CYS | A | 25 | -0.996 | 52.522 | 45.815 | 1.00 | 34.57  |
| ATOM | 186 | O   | CYS | A | 25 | 0.030  | 52.676 | 45.100 | 1.00 | 30.46  |
| ATOM | 187 | CB  | CYS | A | 25 | -1.599 | 50.732 | 47.481 | 1.00 | 37.45  |
| ATOM | 188 | SG  | CYS | A | 25 | 0.119  | 50.641 | 48.047 | 1.00 | 41.07  |
| ATOM | 189 | N   | SER | A | 26 | -1.606 | 53.493 | 46.507 | 1.00 | 32.19  |
| ATOM | 190 | CA  | SER | A | 26 | -1.098 | 54.841 | 46.486 | 1.00 | 32.91  |
| ATOM | 191 | C   | SER | A | 26 | -0.861 | 55.372 | 47.877 | 1.00 | 28.73  |
| ATOM | 192 | O   | SER | A | 26 | -1.638 | 55.107 | 48.802 | 1.00 | 24.93  |
| ATOM | 193 | CB  | SER | A | 26 | -1.884 | 55.825 | 45.626 | 1.00 | 41.21  |
| ATOM | 194 | OG  | SER | A | 26 | -0.987 | 56.748 | 45.012 | 1.00 | 55.61  |
| ATOM | 195 | N   | VAL | A | 27 | 0.258  | 56.092 | 47.964 | 1.00 | 28.06  |
| ATOM | 196 | CA  | VAL | A | 27 | 0.719  | 56.718 | 49.172 | 1.00 | 29.85  |
| ATOM | 197 | C   | VAL | A | 27 | 0.330  | 58.199 | 49.211 | 1.00 | 33.50  |
| ATOM | 198 | O   | VAL | A | 27 | 0.868  | 59.024 | 48.443 | 1.00 | 31.85  |
| ATOM | 199 | CB  | VAL | A | 27 | 2.217  | 56.509 | 49.370 | 1.00 | 34.37  |
| ATOM | 200 | CG1 | VAL | A | 27 | 2.605  | 57.003 | 50.774 | 1.00 | 35.81  |
| ATOM | 201 | CG2 | VAL | A | 27 | 2.481  | 55.004 | 49.263 | 1.00 | 33.03  |
| ATOM | 202 | N   | ASP | A | 28 | -0.626 | 58.489 | 50.106 | 1.00 | 31.46  |
| ATOM | 203 | CA  | ASP | A | 28 | -1.137 | 59.841 | 50.327 | 1.00 | 32.29  |
| ATOM | 204 | C   | ASP | A | 28 | -0.700 | 60.403 | 51.687 | 1.00 | 27.74  |
| ATOM | 205 | O   | ASP | A | 28 | -1.254 | 60.057 | 52.728 | 1.00 | 25.85  |
| ATOM | 206 | CB  | ASP | A | 28 | -2.663 | 59.943 | 50.144 | 1.00 | 35.45  |
| ATOM | 207 | CG  | ASP | A | 28 | -3.158 | 61.380 | 50.016 | 1.00 | 43.54  |
| ATOM | 208 | OD1 | ASP | A | 28 | -2.559 | 62.348 | 50.463 | 1.00 | 39.89  |
| ATOM | 209 | OD2 | ASP | A | 28 | -4.290 | 61.467 | 49.353 | 1.00 | 50.90  |
| ATOM | 210 | N   | PHE | A | 29 | 0.311  | 61.251 | 51.614 | 1.00 | 29.04  |
| ATOM | 211 | CA  | PHE | A | 29 | 0.913  | 61.918 | 52.741 | 1.00 | 32.69  |
| ATOM | 212 | C   | PHE | A | 29 | 0.011  | 63.004 | 53.317 | 1.00 | 46.23  |
| ATOM |     |     |     |   |    |        |        |        |      |        |



|      |     |     |     |   |    |        |        |        |      |       |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|
| ATOM | 227 | CG2 | THR | A | 30 | -3.634 | 65.886 | 51.979 | 1.00 | 42.00 |
| ATOM | 228 | N   | ARG | A | 31 | -3.249 | 62.803 | 53.426 | 1.00 | 23.27 |
| ATOM | 229 | CA  | ARG | A | 31 | -4.258 | 62.179 | 54.263 | 1.00 | 22.52 |
| ATOM | 230 | C   | ARG | A | 31 | -3.670 | 61.084 | 55.187 | 1.00 | 28.33 |
| ATOM | 231 | O   | ARG | A | 31 | -4.388 | 60.485 | 56.013 | 1.00 | 26.36 |
| ATOM | 232 | CB  | ARG | A | 31 | -5.360 | 61.545 | 53.423 | 1.00 | 29.16 |
| ATOM | 233 | CG  | ARG | A | 31 | -6.236 | 62.579 | 52.723 | 1.00 | 52.89 |
| ATOM | 234 | CD  | ARG | A | 31 | -6.324 | 62.368 | 51.215 | 1.00 | 63.14 |
| ATOM | 235 | NE  | ARG | A | 31 | -5.912 | 63.537 | 50.434 | 1.00 | 56.84 |
| ATOM | 236 | CZ  | ARG | A | 31 | -6.777 | 64.353 | 49.868 | 1.00 | 58.33 |
| ATOM | 237 | NH1 | ARG | A | 31 | -8.084 | 64.154 | 49.996 | 1.00 | 45.96 |
| ATOM | 238 | NH2 | ARG | A | 31 | -6.335 | 65.393 | 49.166 | 1.00 | 57.96 |
| ATOM | 239 | N   | ARG | A | 32 | -2.353 | 60.838 | 55.018 | 1.00 | 28.39 |
| ATOM | 240 | CA  | ARG | A | 32 | -1.587 | 59.832 | 55.754 | 1.00 | 28.42 |
| ATOM | 241 | C   | ARG | A | 32 | -2.248 | 58.498 | 55.548 | 1.00 | 31.13 |
| ATOM | 242 | O   | ARG | A | 32 | -2.553 | 57.754 | 56.484 | 1.00 | 26.52 |
| ATOM | 243 | CB  | ARG | A | 32 | -1.353 | 60.163 | 57.233 | 1.00 | 22.96 |
| ATOM | 244 | CG  | ARG | A | 32 | -1.083 | 61.654 | 57.442 | 1.00 | 46.47 |
| ATOM | 245 | CD  | ARG | A | 32 | 0.247  | 62.022 | 58.108 | 1.00 | 65.92 |
| ATOM | 246 | NE  | ARG | A | 32 | 0.307  | 61.670 | 59.532 | 1.00 | 62.95 |
| ATOM | 247 | CZ  | ARG | A | 32 | 1.244  | 62.060 | 60.403 | 1.00 | 56.24 |
| ATOM | 248 | NH1 | ARG | A | 32 | 2.259  | 62.862 | 60.090 | 1.00 | 38.45 |
| ATOM | 249 | NH2 | ARG | A | 32 | 1.150  | 61.628 | 61.644 | 1.00 | 38.26 |
| ATOM | 250 | N   | THR | A | 33 | -2.503 | 58.222 | 54.278 | 1.00 | 30.15 |
| ATOM | 251 | CA  | THR | A | 33 | -3.148 | 56.969 | 53.940 | 1.00 | 30.69 |
| ATOM | 252 | C   | THR | A | 33 | -2.460 | 56.247 | 52.816 | 1.00 | 30.70 |
| ATOM | 253 | O   | THR | A | 33 | -1.765 | 56.842 | 51.978 | 1.00 | 27.23 |
| ATOM | 254 | CB  | THR | A | 33 | -4.603 | 57.146 | 53.467 | 1.00 | 39.23 |
| ATOM | 255 | OG1 | THR | A | 33 | -4.637 | 58.100 | 52.420 | 1.00 | 37.97 |
| ATOM | 256 | CG2 | THR | A | 33 | -5.567 | 57.481 | 54.598 | 1.00 | 34.16 |
| ATOM | 257 | N   | LEU | A | 34 | -2.719 | 54.950 | 52.842 | 1.00 | 30.87 |
| ATOM | 258 | CA  | LEU | A | 34 | -2.279 | 54.012 | 51.842 | 1.00 | 32.01 |
| ATOM | 259 | C   | LEU | A | 34 | -3.598 | 53.483 | 51.332 | 1.00 | 26.54 |
| ATOM | 260 | O   | LEU | A | 34 | -4.426 | 53.031 | 52.106 | 1.00 | 25.08 |
| ATOM | 261 | CB  | LEU | A | 34 | -1.518 | 52.805 | 52.428 | 1.00 | 35.05 |
| ATOM | 262 | CG  | LEU | A | 34 | -0.007 | 52.880 | 52.357 | 1.00 | 42.66 |
| ATOM | 263 | CD1 | LEU | A | 34 | 0.537  | 51.446 | 52.425 | 1.00 | 41.75 |
| ATOM | 264 | CD2 | LEU | A | 34 | 0.434  | 53.610 | 51.081 | 1.00 | 49.07 |
| ATOM | 265 | N   | THR | A | 35 | -3.828 | 53.576 | 50.050 | 1.00 | 27.44 |
| ATOM | 266 | CA  | THR | A | 35 | -5.088 | 53.081 | 49.552 | 1.00 | 29.43 |
| ATOM | 267 | C   | THR | A | 35 | -4.825 | 52.257 | 48.316 | 1.00 | 33.69 |
| ATOM | 268 | O   | THR | A | 35 | -3.896 | 52.559 | 47.532 | 1.00 | 31.06 |
| ATOM | 269 | CB  | THR | A | 35 | -6.004 | 54.248 | 49.195 | 1.00 | 49.67 |
| ATOM | 270 | OG1 | THR | A | 35 | -5.775 | 55.297 | 50.111 | 1.00 | 56.12 |
| ATOM | 271 | CG2 | THR | A | 35 | -7.442 | 53.781 | 49.282 | 1.00 | 53.32 |
| ATOM | 272 | N   | GLY | A | 36 | -5.638 | 51.220 | 48.172 | 1.00 | 31.25 |
| ATOM | 273 | CA  | GLY | A | 36 | -5.509 | 50.336 | 47.024 | 1.00 | 30.78 |
| ATOM | 274 | C   | GLY | A | 36 | -6.314 | 49.072 | 47.144 | 1.00 | 27.36 |
| ATOM | 275 | O   | GLY | A | 36 | -7.358 | 48.969 | 47.773 | 1.00 | 26.53 |
| ATOM | 276 | N   | THR | A | 37 | -5.809 | 48.080 | 46.504 | 1.00 | 27.32 |
| ATOM | 277 | CA  | THR | A | 37 | -6.478 | 46.793 | 46.579 | 1.00 | 29.08 |
| ATOM | 278 | C   | THR | A | 37 | -5.460 | 45.717 | 46.846 | 1.00 | 29.62 |
| ATOM | 279 | O   | THR | A | 37 | -4.321 | 45.787 | 46.370 | 1.00 | 27.85 |
| ATOM | 280 | CB  | THR | A | 37 | -7.268 | 46.425 | 45.311 | 1.00 | 35.94 |
| ATOM | 281 | OG1 | THR | A | 37 | -6.546 | 46.790 | 44.142 | 1.00 | 33.45 |
| ATOM | 282 | CG2 | THR | A | 37 | -8.601 | 47.144 | 45.350 | 1.00 | 41.23 |
| ATOM | 283 | N   | ALA | A | 38 | -5.867 | 44.738 | 47.609 | 1.00 | 28.10 |
| ATOM | 284 | CA  | ALA | A | 38 | -4.934 | 43.674 | 47.856 | 1.00 | 27.55 |



|      |     |     |     |   |    |         |        |        |      |       |
|------|-----|-----|-----|---|----|---------|--------|--------|------|-------|
| ATOM | 285 | C   | ALA | A | 38 | -5.482  | 42.447 | 47.137 | 1.00 | 30.70 |
| ATOM | 286 | O   | ALA | A | 38 | -6.536  | 41.941 | 47.510 | 1.00 | 31.51 |
| ATOM | 287 | CB  | ALA | A | 38 | -4.803  | 43.425 | 49.339 | 1.00 | 26.00 |
| ATOM | 288 | N   | ALA | A | 39 | -4.798  | 41.981 | 46.090 | 1.00 | 27.63 |
| ATOM | 289 | CA  | ALA | A | 39 | -5.280  | 40.761 | 45.394 | 1.00 | 29.40 |
| ATOM | 290 | C   | ALA | A | 39 | -4.563  | 39.541 | 45.966 | 1.00 | 29.05 |
| ATOM | 291 | O   | ALA | A | 39 | -3.371  | 39.333 | 45.734 | 1.00 | 28.04 |
| ATOM | 292 | CB  | ALA | A | 39 | -5.024  | 40.787 | 43.888 | 1.00 | 30.14 |
| ATOM | 293 | N   | LEU | A | 40 | -5.327  | 38.780 | 46.713 | 1.00 | 26.03 |
| ATOM | 294 | CA  | LEU | A | 40 | -4.899  | 37.591 | 47.392 | 1.00 | 26.04 |
| ATOM | 295 | C   | LEU | A | 40 | -5.304  | 36.310 | 46.637 | 1.00 | 30.62 |
| ATOM | 296 | O   | LEU | A | 40 | -6.499  | 36.038 | 46.394 | 1.00 | 28.36 |
| ATOM | 297 | CB  | LEU | A | 40 | -5.596  | 37.499 | 48.779 | 1.00 | 24.92 |
| ATOM | 298 | CG  | LEU | A | 40 | -5.312  | 38.663 | 49.725 | 1.00 | 27.54 |
| ATOM | 299 | CD1 | LEU | A | 40 | -5.870  | 38.272 | 51.074 | 1.00 | 29.18 |
| ATOM | 300 | CD2 | LEU | A | 40 | -3.817  | 38.865 | 49.857 | 1.00 | 26.20 |
| ATOM | 301 | N   | THR | A | 41 | -4.302  | 35.498 | 46.326 | 1.00 | 23.66 |
| ATOM | 302 | CA  | THR | A | 41 | -4.566  | 34.232 | 45.700 | 1.00 | 23.84 |
| ATOM | 303 | C   | THR | A | 41 | -4.509  | 33.259 | 46.841 | 1.00 | 28.24 |
| ATOM | 304 | O   | THR | A | 41 | -3.448  | 33.076 | 47.421 | 1.00 | 28.49 |
| ATOM | 305 | CB  | THR | A | 41 | -3.554  | 33.854 | 44.613 | 1.00 | 38.89 |
| ATOM | 306 | OG1 | THR | A | 41 | -3.594  | 34.801 | 43.555 | 1.00 | 32.11 |
| ATOM | 307 | CG2 | THR | A | 41 | -3.856  | 32.426 | 44.113 | 1.00 | 33.97 |
| ATOM | 308 | N   | VAL | A | 42 | -5.674  | 32.704 | 47.169 | 1.00 | 25.76 |
| ATOM | 309 | CA  | VAL | A | 42 | -5.843  | 31.782 | 48.261 | 1.00 | 26.45 |
| ATOM | 310 | C   | VAL | A | 42 | -6.068  | 30.356 | 47.804 | 1.00 | 34.04 |
| ATOM | 311 | O   | VAL | A | 42 | -6.730  | 30.118 | 46.795 | 1.00 | 33.15 |
| ATOM | 312 | CB  | VAL | A | 42 | -7.024  | 32.223 | 49.113 | 1.00 | 29.66 |
| ATOM | 313 | CG1 | VAL | A | 42 | -7.189  | 31.274 | 50.295 | 1.00 | 30.14 |
| ATOM | 314 | CG2 | VAL | A | 42 | -6.805  | 33.657 | 49.611 | 1.00 | 28.98 |
| ATOM | 315 | N   | GLN | A | 43 | -5.530  | 29.405 | 48.566 | 1.00 | 29.23 |
| ATOM | 316 | CA  | GLN | A | 43 | -5.692  | 27.989 | 48.247 | 1.00 | 28.15 |
| ATOM | 317 | C   | GLN | A | 43 | -6.357  | 27.171 | 49.356 | 1.00 | 31.60 |
| ATOM | 318 | O   | GLN | A | 43 | -5.916  | 27.081 | 50.506 | 1.00 | 30.09 |
| ATOM | 319 | CB  | GLN | A | 43 | -4.401  | 27.337 | 47.748 | 1.00 | 29.76 |
| ATOM | 320 | CG  | GLN | A | 43 | -4.305  | 25.877 | 48.214 | 1.00 | 49.25 |
| ATOM | 321 | CD  | GLN | A | 43 | -2.920  | 25.308 | 48.018 | 1.00 | 68.40 |
| ATOM | 322 | OE1 | GLN | A | 43 | -2.508  | 25.059 | 46.882 | 1.00 | 65.93 |
| ATOM | 323 | NE2 | GLN | A | 43 | -2.190  | 25.118 | 49.116 | 1.00 | 62.52 |
| ATOM | 324 | N   | SER | A | 44 | -7.470  | 26.553 | 49.027 | 1.00 | 25.74 |
| ATOM | 325 | CA  | SER | A | 44 | -8.159  | 25.793 | 50.027 | 1.00 | 24.21 |
| ATOM | 326 | C   | SER | A | 44 | -7.406  | 24.562 | 50.434 | 1.00 | 31.27 |
| ATOM | 327 | O   | SER | A | 44 | -6.701  | 23.950 | 49.642 | 1.00 | 33.21 |
| ATOM | 328 | CB  | SER | A | 44 | -9.542  | 25.400 | 49.574 | 1.00 | 28.22 |
| ATOM | 329 | OG  | SER | A | 44 | -10.143 | 24.569 | 50.550 | 1.00 | 36.23 |
| ATOM | 330 | N   | GLN | A | 45 | -7.593  | 24.190 | 51.685 | 1.00 | 29.25 |
| ATOM | 331 | CA  | GLN | A | 45 | -6.964  | 23.016 | 52.240 | 1.00 | 32.48 |
| ATOM | 332 | C   | GLN | A | 45 | -8.027  | 22.007 | 52.618 | 1.00 | 41.18 |
| ATOM | 333 | O   | GLN | A | 45 | -7.757  | 20.936 | 53.165 | 1.00 | 37.68 |
| ATOM | 334 | CB  | GLN | A | 45 | -6.095  | 23.387 | 53.451 | 1.00 | 35.17 |
| ATOM | 335 | CG  | GLN | A | 45 | -5.138  | 24.525 | 53.090 | 1.00 | 29.17 |
| ATOM | 336 | CD  | GLN | A | 45 | -4.197  | 24.179 | 51.954 | 1.00 | 37.50 |
| ATOM | 337 | OE1 | GLN | A | 45 | -4.107  | 24.903 | 50.939 | 1.00 | 44.48 |
| ATOM | 338 | NE2 | GLN | A | 45 | -3.466  | 23.083 | 52.127 | 1.00 | 23.35 |
| ATOM | 339 | N   | GLU | A | 46 | -9.258  | 22.387 | 52.322 | 1.00 | 40.69 |
| ATOM | 340 | CA  | GLU | A | 46 | -10.391 | 21.548 | 52.591 | 1.00 | 41.85 |
| ATOM | 341 | C   | GLU | A | 46 | -11.311 | 21.472 | 51.388 | 1.00 | 46.94 |
| ATOM | 342 | O   | GLU | A | 46 | -11.146 | 22.143 | 50.367 | 1.00 | 45.45 |



|      |     |     |     |   |    |         |        |        |      |        |
|------|-----|-----|-----|---|----|---------|--------|--------|------|--------|
| ATOM | 343 | CB  | GLU | A | 46 | -11.216 | 21.989 | 53.827 | 1.00 | 42.82  |
| ATOM | 344 | CG  | GLU | A | 46 | -10.736 | 23.256 | 54.548 | 1.00 | 48.14  |
| ATOM | 345 | CD  | GLU | A | 46 | -11.469 | 23.463 | 55.856 | 1.00 | 62.06  |
| ATOM | 346 | OE1 | GLU | A | 46 | -12.507 | 24.103 | 55.957 | 1.00 | 64.38  |
| ATOM | 347 | OE2 | GLU | A | 46 | -10.880 | 22.875 | 56.871 | 1.00 | 51.57  |
| ATOM | 348 | N   | ASP | A | 47 | -12.306 | 20.638 | 51.523 | 1.00 | 46.70  |
| ATOM | 349 | CA  | ASP | A | 47 | -13.261 | 20.543 | 50.464 | 1.00 | 48.51  |
| ATOM | 350 | C   | ASP | A | 47 | -14.408 | 21.358 | 50.947 | 1.00 | 45.90  |
| ATOM | 351 | O   | ASP | A | 47 | -14.674 | 21.368 | 52.148 | 1.00 | 41.55  |
| ATOM | 352 | CB  | ASP | A | 47 | -13.748 | 19.104 | 50.220 | 1.00 | 52.32  |
| ATOM | 353 | CG  | ASP | A | 47 | -12.739 | 18.258 | 49.495 | 1.00 | 80.62  |
| ATOM | 354 | OD1 | ASP | A | 47 | -12.338 | 18.505 | 48.364 | 1.00 | 77.22  |
| ATOM | 355 | OD2 | ASP | A | 47 | -12.330 | 17.237 | 50.218 | 1.00 | 100.00 |
| ATOM | 356 | N   | ASN | A | 48 | -15.067 | 22.044 | 50.045 | 1.00 | 44.45  |
| ATOM | 357 | CA  | ASN | A | 48 | -16.209 | 22.826 | 50.475 | 1.00 | 45.83  |
| ATOM | 358 | C   | ASN | A | 48 | -15.875 | 24.055 | 51.308 | 1.00 | 46.95  |
| ATOM | 359 | O   | ASN | A | 48 | -16.620 | 24.449 | 52.219 | 1.00 | 45.85  |
| ATOM | 360 | CB  | ASN | A | 48 | -17.246 | 21.959 | 51.225 | 1.00 | 43.60  |
| ATOM | 361 | CG  | ASN | A | 48 | -18.653 | 22.469 | 51.004 | 1.00 | 65.69  |
| ATOM | 362 | OD1 | ASN | A | 48 | -18.924 | 23.191 | 50.027 | 1.00 | 68.02  |
| ATOM | 363 | ND2 | ASN | A | 48 | -19.545 | 22.123 | 51.922 | 1.00 | 53.94  |
| ATOM | 364 | N   | LEU | A | 49 | -14.758 | 24.672 | 51.004 | 1.00 | 40.04  |
| ATOM | 365 | CA  | LEU | A | 49 | -14.445 | 25.850 | 51.741 | 1.00 | 35.92  |
| ATOM | 366 | C   | LEU | A | 49 | -15.377 | 26.909 | 51.178 | 1.00 | 39.46  |
| ATOM | 367 | O   | LEU | A | 49 | -15.301 | 27.241 | 49.998 | 1.00 | 36.67  |
| ATOM | 368 | CB  | LEU | A | 49 | -12.977 | 26.218 | 51.556 | 1.00 | 34.20  |
| ATOM | 369 | CG  | LEU | A | 49 | -12.623 | 27.492 | 52.307 | 1.00 | 36.68  |
| ATOM | 370 | CD1 | LEU | A | 49 | -13.000 | 27.286 | 53.753 | 1.00 | 35.00  |
| ATOM | 371 | CD2 | LEU | A | 49 | -11.135 | 27.785 | 52.181 | 1.00 | 38.84  |
| ATOM | 372 | N   | ARG | A | 50 | -16.287 | 27.411 | 51.998 | 1.00 | 40.21  |
| ATOM | 373 | CA  | ARG | A | 50 | -17.242 | 28.417 | 51.525 | 1.00 | 41.40  |
| ATOM | 374 | C   | ARG | A | 50 | -16.907 | 29.859 | 51.901 | 1.00 | 47.29  |
| ATOM | 375 | O   | ARG | A | 50 | -17.364 | 30.801 | 51.263 | 1.00 | 47.10  |
| ATOM | 376 | CB  | ARG | A | 50 | -18.644 | 28.046 | 51.980 | 1.00 | 38.23  |
| ATOM | 377 | CG  | ARG | A | 50 | -18.911 | 26.547 | 51.811 | 1.00 | 52.44  |
| ATOM | 378 | CD  | ARG | A | 50 | -20.385 | 26.171 | 51.839 | 1.00 | 58.37  |
| ATOM | 379 | NE  | ARG | A | 50 | -20.835 | 25.461 | 50.643 | 1.00 | 80.87  |
| ATOM | 380 | CZ  | ARG | A | 50 | -21.951 | 24.727 | 50.592 | 1.00 | 100.00 |
| ATOM | 381 | NH1 | ARG | A | 50 | -22.750 | 24.575 | 51.652 | 1.00 | 100.00 |
| ATOM | 382 | NH2 | ARG | A | 50 | -22.272 | 24.127 | 49.446 | 1.00 | 65.83  |
| ATOM | 383 | N   | SER | A | 51 | -16.102 | 30.024 | 52.945 | 1.00 | 43.64  |
| ATOM | 384 | CA  | SER | A | 51 | -15.714 | 31.334 | 53.418 | 1.00 | 41.14  |
| ATOM | 385 | C   | SER | A | 51 | -14.454 | 31.283 | 54.259 | 1.00 | 44.29  |
| ATOM | 386 | O   | SER | A | 51 | -14.253 | 30.319 | 55.016 | 1.00 | 46.38  |
| ATOM | 387 | CB  | SER | A | 51 | -16.821 | 31.863 | 54.321 | 1.00 | 45.40  |
| ATOM | 388 | OG  | SER | A | 51 | -16.862 | 31.143 | 55.556 | 1.00 | 46.27  |
| ATOM | 389 | N   | LEU | A | 52 | -13.623 | 32.330 | 54.156 | 1.00 | 36.51  |
| ATOM | 390 | CA  | LEU | A | 52 | -12.418 | 32.411 | 54.964 | 1.00 | 36.39  |
| ATOM | 391 | C   | LEU | A | 52 | -12.369 | 33.667 | 55.852 | 1.00 | 42.80  |
| ATOM | 392 | O   | LEU | A | 52 | -13.113 | 34.644 | 55.647 | 1.00 | 40.92  |
| ATOM | 393 | CB  | LEU | A | 52 | -11.103 | 32.143 | 54.203 | 1.00 | 35.84  |
| ATOM | 394 | CG  | LEU | A | 52 | -10.729 | 33.115 | 53.095 | 1.00 | 39.41  |
| ATOM | 395 | CD1 | LEU | A | 52 | -11.745 | 33.042 | 51.994 | 1.00 | 41.33  |
| ATOM | 396 | CD2 | LEU | A | 52 | -10.624 | 34.538 | 53.605 | 1.00 | 38.19  |
| ATOM | 397 | N   | VAL | A | 53 | -11.491 | 33.659 | 56.859 | 1.00 | 37.98  |
| ATOM | 398 | CA  | VAL | A | 53 | -11.331 | 34.834 | 57.737 | 1.00 | 34.43  |
| ATOM | 399 | C   | VAL | A | 53 | -9.933  | 35.384 | 57.550 | 1.00 | 31.66  |
| ATOM | 400 | O   | VAL | A | 53 | -8.975  | 34.606 | 57.511 | 1.00 | 28.02  |



|      |     |     |     |   |    |         |        |        |      |       |
|------|-----|-----|-----|---|----|---------|--------|--------|------|-------|
| ATOM | 401 | CB  | VAL | A | 53 | -11.601 | 34.597 | 59.226 | 1.00 | 37.95 |
| ATOM | 402 | CG1 | VAL | A | 53 | -11.580 | 35.929 | 59.989 | 1.00 | 37.38 |
| ATOM | 403 | CG2 | VAL | A | 53 | -12.946 | 33.922 | 59.419 | 1.00 | 37.84 |
| ATOM | 404 | N   | LEU | A | 54 | -9.829  | 36.705 | 57.418 | 1.00 | 23.95 |
| ATOM | 405 | CA  | LEU | A | 54 | -8.558  | 37.365 | 57.270 | 1.00 | 22.89 |
| ATOM | 406 | C   | LEU | A | 54 | -8.395  | 38.285 | 58.470 | 1.00 | 29.33 |
| ATOM | 407 | O   | LEU | A | 54 | -9.388  | 38.613 | 59.138 | 1.00 | 25.65 |
| ATOM | 408 | CB  | LEU | A | 54 | -8.515  | 38.242 | 56.019 | 1.00 | 23.57 |
| ATOM | 409 | CG  | LEU | A | 54 | -8.458  | 37.469 | 54.700 | 1.00 | 32.01 |
| ATOM | 410 | CD1 | LEU | A | 54 | -8.345  | 38.475 | 53.541 | 1.00 | 31.66 |
| ATOM | 411 | CD2 | LEU | A | 54 | -7.271  | 36.505 | 54.684 | 1.00 | 24.96 |
| ATOM | 412 | N   | ASP | A | 55 | -7.145  | 38.698 | 58.732 | 1.00 | 28.72 |
| ATOM | 413 | CA  | ASP | A | 55 | -6.830  | 39.616 | 59.831 | 1.00 | 24.54 |
| ATOM | 414 | C   | ASP | A | 55 | -6.845  | 41.043 | 59.289 | 1.00 | 22.50 |
| ATOM | 415 | O   | ASP | A | 55 | -6.460  | 41.312 | 58.173 | 1.00 | 21.41 |
| ATOM | 416 | CB  | ASP | A | 55 | -5.446  | 39.344 | 60.500 | 1.00 | 25.99 |
| ATOM | 417 | CG  | ASP | A | 55 | -5.298  | 38.132 | 61.418 | 1.00 | 23.16 |
| ATOM | 418 | OD1 | ASP | A | 55 | -5.887  | 37.985 | 62.470 | 1.00 | 27.99 |
| ATOM | 419 | OD2 | ASP | A | 55 | -4.408  | 37.248 | 60.991 | 1.00 | 24.58 |
| ATOM | 420 | N   | THR | A | 56 | -7.309  | 41.977 | 60.109 | 1.00 | 21.37 |
| ATOM | 421 | CA  | THR | A | 56 | -7.346  | 43.373 | 59.748 | 1.00 | 22.34 |
| ATOM | 422 | C   | THR | A | 56 | -7.167  | 44.196 | 61.019 | 1.00 | 25.71 |
| ATOM | 423 | O   | THR | A | 56 | -7.573  | 43.726 | 62.088 | 1.00 | 26.22 |
| ATOM | 424 | CB  | THR | A | 56 | -8.727  | 43.717 | 59.133 | 1.00 | 34.75 |
| ATOM | 425 | OG1 | THR | A | 56 | -9.668  | 43.936 | 60.183 | 1.00 | 35.02 |
| ATOM | 426 | CG2 | THR | A | 56 | -9.210  | 42.578 | 58.241 | 1.00 | 40.12 |
| ATOM | 427 | N   | LYS | A | 57 | -6.598  | 45.405 | 60.918 | 1.00 | 20.41 |
| ATOM | 428 | CA  | LYS | A | 57 | -6.478  | 46.239 | 62.114 | 1.00 | 19.63 |
| ATOM | 429 | C   | LYS | A | 57 | -6.656  | 47.686 | 61.717 | 1.00 | 21.21 |
| ATOM | 430 | O   | LYS | A | 57 | -5.851  | 48.222 | 60.995 | 1.00 | 19.18 |
| ATOM | 431 | CB  | LYS | A | 57 | -5.182  | 45.983 | 62.827 | 1.00 | 21.05 |
| ATOM | 432 | CG  | LYS | A | 57 | -5.137  | 46.424 | 64.271 | 1.00 | 26.38 |
| ATOM | 433 | CD  | LYS | A | 57 | -3.713  | 46.855 | 64.626 | 1.00 | 44.32 |
| ATOM | 434 | CE  | LYS | A | 57 | -3.331  | 46.750 | 66.099 | 1.00 | 61.77 |
| ATOM | 435 | NZ  | LYS | A | 57 | -1.996  | 47.313 | 66.396 | 1.00 | 53.68 |
| ATOM | 436 | N   | ASP | A | 58 | -7.739  | 48.322 | 62.162 | 1.00 | 23.32 |
| ATOM | 437 | CA  | ASP | A | 58 | -7.952  | 49.707 | 61.772 | 1.00 | 22.42 |
| ATOM | 438 | C   | ASP | A | 58 | -7.930  | 49.875 | 60.266 | 1.00 | 27.00 |
| ATOM | 439 | O   | ASP | A | 58 | -7.376  | 50.808 | 59.668 | 1.00 | 24.72 |
| ATOM | 440 | CB  | ASP | A | 58 | -6.971  | 50.657 | 62.459 | 1.00 | 24.48 |
| ATOM | 441 | CG  | ASP | A | 58 | -7.104  | 50.494 | 63.928 | 1.00 | 36.08 |
| ATOM | 442 | OD1 | ASP | A | 58 | -8.187  | 50.358 | 64.474 | 1.00 | 38.70 |
| ATOM | 443 | OD2 | ASP | A | 58 | -5.944  | 50.459 | 64.535 | 1.00 | 37.78 |
| ATOM | 444 | N   | LEU | A | 59 | -8.530  | 48.936 | 59.611 | 1.00 | 26.57 |
| ATOM | 445 | CA  | LEU | A | 59 | -8.545  | 49.049 | 58.177 | 1.00 | 26.97 |
| ATOM | 446 | C   | LEU | A | 59 | -9.946  | 49.473 | 57.707 | 1.00 | 30.09 |
| ATOM | 447 | O   | LEU | A | 59 | -10.971 | 49.074 | 58.245 | 1.00 | 28.07 |
| ATOM | 448 | CB  | LEU | A | 59 | -8.132  | 47.698 | 57.479 | 1.00 | 26.65 |
| ATOM | 449 | CG  | LEU | A | 59 | -6.639  | 47.356 | 57.443 | 1.00 | 24.34 |
| ATOM | 450 | CD1 | LEU | A | 59 | -6.445  | 46.049 | 56.687 | 1.00 | 25.03 |
| ATOM | 451 | CD2 | LEU | A | 59 | -5.864  | 48.443 | 56.722 | 1.00 | 21.60 |
| ATOM | 452 | N   | THR | A | 60 | -9.982  | 50.278 | 56.673 | 1.00 | 29.73 |
| ATOM | 453 | CA  | THR | A | 60 | -11.244 | 50.685 | 56.091 | 1.00 | 30.53 |
| ATOM | 454 | C   | THR | A | 60 | -11.433 | 49.876 | 54.791 | 1.00 | 34.07 |
| ATOM | 455 | O   | THR | A | 60 | -10.634 | 49.978 | 53.813 | 1.00 | 29.18 |
| ATOM | 456 | CB  | THR | A | 60 | -11.282 | 52.198 | 55.881 | 1.00 | 38.77 |
| ATOM | 457 | OG1 | THR | A | 60 | -11.898 | 52.759 | 57.020 | 1.00 | 55.62 |
| ATOM | 458 | CG2 | THR | A | 60 | -12.086 | 52.528 | 54.635 | 1.00 | 42.40 |



60123410-023699

|      |     |     |     |   |    |         |        |        |      |        |
|------|-----|-----|-----|---|----|---------|--------|--------|------|--------|
| ATOM | 459 | N   | ILE | A | 61 | -12.465 | 49.042 | 54.808 | 1.00 | 30.99  |
| ATOM | 460 | CA  | ILE | A | 61 | -12.758 | 48.181 | 53.667 | 1.00 | 33.20  |
| ATOM | 461 | C   | ILE | A | 61 | -13.821 | 48.708 | 52.741 | 1.00 | 38.63  |
| ATOM | 462 | O   | ILE | A | 61 | -14.987 | 48.694 | 53.102 | 1.00 | 34.56  |
| ATOM | 463 | CB  | ILE | A | 61 | -13.230 | 46.809 | 54.087 | 1.00 | 37.17  |
| ATOM | 464 | CG1 | ILE | A | 61 | -12.407 | 46.229 | 55.252 | 1.00 | 37.33  |
| ATOM | 465 | CG2 | ILE | A | 61 | -13.229 | 45.905 | 52.850 | 1.00 | 39.90  |
| ATOM | 466 | CD1 | ILE | A | 61 | -10.929 | 46.003 | 54.937 | 1.00 | 41.79  |
| ATOM | 467 | N   | GLU | A | 62 | -13.407 | 49.117 | 51.548 | 1.00 | 42.13  |
| ATOM | 468 | CA  | GLU | A | 62 | -14.330 | 49.624 | 50.543 | 1.00 | 45.12  |
| ATOM | 469 | C   | GLU | A | 62 | -15.208 | 48.498 | 49.976 | 1.00 | 48.64  |
| ATOM | 470 | O   | GLU | A | 62 | -16.442 | 48.537 | 49.984 | 1.00 | 49.46  |
| ATOM | 471 | CB  | GLU | A | 62 | -13.550 | 50.305 | 49.397 | 1.00 | 47.88  |
| ATOM | 472 | CG  | GLU | A | 62 | -14.390 | 51.345 | 48.620 | 1.00 | 73.90  |
| ATOM | 473 | CD  | GLU | A | 62 | -15.062 | 50.839 | 47.363 | 1.00 | 100.00 |
| ATOM | 474 | OE1 | GLU | A | 62 | -16.062 | 50.129 | 47.371 | 1.00 | 100.00 |
| ATOM | 475 | OE2 | GLU | A | 62 | -14.492 | 51.296 | 46.267 | 1.00 | 100.00 |
| ATOM | 476 | N   | LYS | A | 63 | -14.551 | 47.459 | 49.483 | 1.00 | 40.80  |
| ATOM | 477 | CA  | LYS | A | 63 | -15.283 | 46.342 | 48.931 | 1.00 | 36.23  |
| ATOM | 478 | C   | LYS | A | 63 | -14.377 | 45.153 | 48.678 | 1.00 | 34.27  |
| ATOM | 479 | O   | LYS | A | 63 | -13.167 | 45.306 | 48.512 | 1.00 | 29.28  |
| ATOM | 480 | CB  | LYS | A | 63 | -15.891 | 46.760 | 47.601 | 1.00 | 32.16  |
| ATOM | 481 | CG  | LYS | A | 63 | -14.816 | 47.067 | 46.573 | 1.00 | 22.38  |
| ATOM | 482 | CD  | LYS | A | 63 | -15.373 | 47.148 | 45.162 | 1.00 | 32.02  |
| ATOM | 483 | CE  | LYS | A | 63 | -14.778 | 48.257 | 44.308 | 1.00 | 33.99  |
| ATOM | 484 | NZ  | LYS | A | 63 | -13.723 | 47.814 | 43.365 | 1.00 | 52.00  |
| ATOM | 485 | N   | VAL | A | 64 | -15.001 | 43.985 | 48.614 | 1.00 | 36.16  |
| ATOM | 486 | CA  | VAL | A | 64 | -14.292 | 42.751 | 48.306 | 1.00 | 39.33  |
| ATOM | 487 | C   | VAL | A | 64 | -14.792 | 42.157 | 46.993 | 1.00 | 43.15  |
| ATOM | 488 | O   | VAL | A | 64 | -15.971 | 41.822 | 46.859 | 1.00 | 38.90  |
| ATOM | 489 | CB  | VAL | A | 64 | -14.401 | 41.692 | 49.370 | 1.00 | 42.66  |
| ATOM | 490 | CG1 | VAL | A | 64 | -13.465 | 40.566 | 48.928 | 1.00 | 42.11  |
| ATOM | 491 | CG2 | VAL | A | 64 | -14.028 | 42.276 | 50.730 | 1.00 | 40.96  |
| ATOM | 492 | N   | VAL | A | 65 | -13.892 | 42.023 | 46.036 | 1.00 | 40.44  |
| ATOM | 493 | CA  | VAL | A | 65 | -14.287 | 41.505 | 44.739 | 1.00 | 37.94  |
| ATOM | 494 | C   | VAL | A | 65 | -13.708 | 40.162 | 44.350 | 1.00 | 35.48  |
| ATOM | 495 | O   | VAL | A | 65 | -12.511 | 39.915 | 44.474 | 1.00 | 31.12  |
| ATOM | 496 | CB  | VAL | A | 65 | -14.047 | 42.540 | 43.647 | 1.00 | 39.44  |
| ATOM | 497 | CG1 | VAL | A | 65 | -14.238 | 41.899 | 42.287 | 1.00 | 38.78  |
| ATOM | 498 | CG2 | VAL | A | 65 | -15.024 | 43.692 | 43.844 | 1.00 | 38.69  |
| ATOM | 499 | N   | ILE | A | 66 | -14.599 | 39.316 | 43.847 | 1.00 | 32.12  |
| ATOM | 500 | CA  | ILE | A | 66 | -14.223 | 38.010 | 43.372 | 1.00 | 31.54  |
| ATOM | 501 | C   | ILE | A | 66 | -14.825 | 37.784 | 41.993 | 1.00 | 37.42  |
| ATOM | 502 | O   | ILE | A | 66 | -16.033 | 37.896 | 41.794 | 1.00 | 34.45  |
| ATOM | 503 | CB  | ILE | A | 66 | -14.602 | 36.884 | 44.313 | 1.00 | 32.82  |
| ATOM | 504 | CG1 | ILE | A | 66 | -13.945 | 37.071 | 45.664 | 1.00 | 30.69  |
| ATOM | 505 | CG2 | ILE | A | 66 | -14.117 | 35.581 | 43.703 | 1.00 | 32.94  |
| ATOM | 506 | CD1 | ILE | A | 66 | -14.478 | 36.125 | 46.731 | 1.00 | 25.31  |
| ATOM | 507 | N   | ASN | A | 67 | -13.968 | 37.498 | 41.027 | 1.00 | 38.89  |
| ATOM | 508 | CA  | ASN | A | 67 | -14.426 | 37.278 | 39.668 | 1.00 | 39.33  |
| ATOM | 509 | C   | ASN | A | 67 | -15.373 | 38.366 | 39.223 | 1.00 | 42.51  |
| ATOM | 510 | O   | ASN | A | 67 | -16.525 | 38.092 | 38.906 | 1.00 | 39.37  |
| ATOM | 511 | CB  | ASN | A | 67 | -15.095 | 35.904 | 39.501 | 1.00 | 35.20  |
| ATOM | 512 | CG  | ASN | A | 67 | -14.141 | 34.765 | 39.862 | 1.00 | 61.24  |
| ATOM | 513 | OD1 | ASN | A | 67 | -12.900 | 34.842 | 39.669 | 1.00 | 47.44  |
| ATOM | 514 | ND2 | ASN | A | 67 | -14.717 | 33.706 | 40.421 | 1.00 | 42.22  |
| ATOM | 515 | N   | GLY | A | 68 | -14.848 | 39.590 | 39.237 | 1.00 | 39.48  |
| ATOM | 516 | CA  | GLY | A | 68 | -15.527 | 40.809 | 38.826 | 1.00 | 37.68  |



50122140 023609

|      |     |     |     |   |    |         |        |        |      |        |
|------|-----|-----|-----|---|----|---------|--------|--------|------|--------|
| ATOM | 517 | C   | GLY | A | 68 | -16.763 | 41.167 | 39.612 | 1.00 | 39.81  |
| ATOM | 518 | O   | GLY | A | 68 | -17.380 | 42.197 | 39.398 | 1.00 | 43.86  |
| ATOM | 519 | N   | GLN | A | 69 | -17.173 | 40.333 | 40.513 | 1.00 | 33.09  |
| ATOM | 520 | CA  | GLN | A | 69 | -18.351 | 40.732 | 41.230 | 1.00 | 34.40  |
| ATOM | 521 | C   | GLN | A | 69 | -17.958 | 41.090 | 42.626 | 1.00 | 47.27  |
| ATOM | 522 | O   | GLN | A | 69 | -16.841 | 40.790 | 43.059 | 1.00 | 49.22  |
| ATOM | 523 | CB  | GLN | A | 69 | -19.416 | 39.624 | 41.285 | 1.00 | 36.28  |
| ATOM | 524 | CG  | GLN | A | 69 | -19.908 | 39.174 | 39.893 | 1.00 | 42.32  |
| ATOM | 525 | CD  | GLN | A | 69 | -20.467 | 40.321 | 39.111 | 1.00 | 54.27  |
| ATOM | 526 | OE1 | GLN | A | 69 | -19.968 | 40.635 | 38.025 | 1.00 | 50.67  |
| ATOM | 527 | NE2 | GLN | A | 69 | -21.462 | 40.989 | 39.696 | 1.00 | 59.09  |
| ATOM | 528 | N   | GLU | A | 70 | -18.898 | 41.715 | 43.318 | 1.00 | 45.54  |
| ATOM | 529 | CA  | GLU | A | 70 | -18.697 | 42.105 | 44.682 | 1.00 | 43.70  |
| ATOM | 530 | C   | GLU | A | 70 | -19.236 | 40.986 | 45.548 | 1.00 | 50.02  |
| ATOM | 531 | O   | GLU | A | 70 | -20.200 | 40.332 | 45.162 | 1.00 | 55.78  |
| ATOM | 532 | CB  | GLU | A | 70 | -19.351 | 43.459 | 44.985 | 1.00 | 43.37  |
| ATOM | 533 | CG  | GLU | A | 70 | -18.528 | 44.659 | 44.476 | 1.00 | 45.21  |
| ATOM | 534 | CD  | GLU | A | 70 | -19.093 | 45.975 | 44.964 | 1.00 | 80.18  |
| ATOM | 535 | OE1 | GLU | A | 70 | -19.937 | 46.064 | 45.861 | 1.00 | 51.66  |
| ATOM | 536 | OE2 | GLU | A | 70 | -18.594 | 47.005 | 44.319 | 1.00 | 79.05  |
| ATOM | 537 | N   | VAL | A | 71 | -18.611 | 40.735 | 46.695 | 1.00 | 37.89  |
| ATOM | 538 | CA  | VAL | A | 71 | -19.067 | 39.666 | 47.551 | 1.00 | 33.11  |
| ATOM | 539 | C   | VAL | A | 71 | -19.420 | 40.129 | 48.963 | 1.00 | 35.14  |
| ATOM | 540 | O   | VAL | A | 71 | -19.165 | 41.257 | 49.380 | 1.00 | 36.32  |
| ATOM | 541 | CB  | VAL | A | 71 | -18.147 | 38.422 | 47.497 | 1.00 | 33.37  |
| ATOM | 542 | CG1 | VAL | A | 71 | -17.772 | 38.119 | 46.050 | 1.00 | 31.13  |
| ATOM | 543 | CG2 | VAL | A | 71 | -16.866 | 38.594 | 48.326 | 1.00 | 31.47  |
| ATOM | 544 | N   | LYS | A | 72 | -20.016 | 39.247 | 49.696 | 1.00 | 31.08  |
| ATOM | 545 | CA  | LYS | A | 72 | -20.385 | 39.549 | 51.037 | 1.00 | 34.55  |
| ATOM | 546 | C   | LYS | A | 72 | -19.155 | 39.360 | 51.922 | 1.00 | 46.45  |
| ATOM | 547 | O   | LYS | A | 72 | -18.344 | 38.455 | 51.678 | 1.00 | 44.93  |
| ATOM | 548 | CB  | LYS | A | 72 | -21.484 | 38.586 | 51.447 | 1.00 | 37.84  |
| ATOM | 549 | CG  | LYS | A | 72 | -22.553 | 39.153 | 52.362 | 1.00 | 60.35  |
| ATOM | 550 | CD  | LYS | A | 72 | -22.630 | 38.370 | 53.660 | 1.00 | 78.18  |
| ATOM | 551 | CE  | LYS | A | 72 | -21.389 | 38.589 | 54.500 | 1.00 | 92.99  |
| ATOM | 552 | NZ  | LYS | A | 72 | -20.860 | 39.935 | 54.295 | 1.00 | 100.00 |
| ATOM | 553 | N   | TYR | A | 73 | -19.051 | 40.242 | 52.930 | 1.00 | 45.41  |
| ATOM | 554 | CA  | TYR | A | 73 | -18.006 | 40.276 | 53.941 | 1.00 | 45.13  |
| ATOM | 555 | C   | TYR | A | 73 | -18.474 | 41.017 | 55.167 | 1.00 | 47.06  |
| ATOM | 556 | O   | TYR | A | 73 | -19.231 | 41.979 | 55.089 | 1.00 | 45.05  |
| ATOM | 557 | CB  | TYR | A | 73 | -16.720 | 40.932 | 53.488 | 1.00 | 44.74  |
| ATOM | 558 | CG  | TYR | A | 73 | -16.753 | 42.438 | 53.504 | 1.00 | 47.77  |
| ATOM | 559 | CD1 | TYR | A | 73 | -16.507 | 43.169 | 54.674 | 1.00 | 50.00  |
| ATOM | 560 | CD2 | TYR | A | 73 | -17.005 | 43.133 | 52.306 | 1.00 | 49.34  |
| ATOM | 561 | CE1 | TYR | A | 73 | -16.519 | 44.565 | 54.662 | 1.00 | 52.06  |
| ATOM | 562 | CE2 | TYR | A | 73 | -16.967 | 44.529 | 52.284 | 1.00 | 50.56  |
| ATOM | 563 | CZ  | TYR | A | 73 | -16.684 | 45.235 | 53.452 | 1.00 | 60.67  |
| ATOM | 564 | OH  | TYR | A | 73 | -16.859 | 46.597 | 53.418 | 1.00 | 66.04  |
| ATOM | 565 | N   | ALA | A | 74 | -17.993 | 40.557 | 56.289 | 1.00 | 40.33  |
| ATOM | 566 | CA  | ALA | A | 74 | -18.323 | 41.138 | 57.545 | 1.00 | 39.85  |
| ATOM | 567 | C   | ALA | A | 74 | -17.068 | 41.281 | 58.412 | 1.00 | 47.89  |
| ATOM | 568 | O   | ALA | A | 74 | -16.147 | 40.464 | 58.346 | 1.00 | 46.81  |
| ATOM | 569 | CB  | ALA | A | 74 | -19.346 | 40.262 | 58.237 | 1.00 | 39.87  |
| ATOM | 570 | N   | LEU | A | 75 | -17.055 | 42.339 | 59.227 | 1.00 | 42.79  |
| ATOM | 571 | CA  | LEU | A | 75 | -15.980 | 42.650 | 60.148 | 1.00 | 38.94  |
| ATOM | 572 | C   | LEU | A | 75 | -16.416 | 42.342 | 61.561 | 1.00 | 44.65  |
| ATOM | 573 | O   | LEU | A | 75 | -17.388 | 42.895 | 62.068 | 1.00 | 48.50  |
| ATOM | 574 | CB  | LEU | A | 75 | -15.667 | 44.141 | 60.115 | 1.00 | 37.30  |



|      |     |     |     |   |    |         |        |        |      |        |
|------|-----|-----|-----|---|----|---------|--------|--------|------|--------|
| ATOM | 575 | CG  | LEU | A | 75 | -14.899 | 44.572 | 58.899 | 1.00 | 44.06  |
| ATOM | 576 | CD1 | LEU | A | 75 | -14.476 | 46.031 | 59.085 | 1.00 | 47.51  |
| ATOM | 577 | CD2 | LEU | A | 75 | -13.691 | 43.666 | 58.677 | 1.00 | 46.54  |
| ATOM | 578 | N   | GLY | A | 76 | -15.718 | 41.474 | 62.242 | 1.00 | 39.16  |
| ATOM | 579 | CA  | GLY | A | 76 | -16.145 | 41.228 | 63.597 | 1.00 | 36.77  |
| ATOM | 580 | C   | GLY | A | 76 | -15.652 | 42.360 | 64.461 | 1.00 | 31.43  |
| ATOM | 581 | O   | GLY | A | 76 | -14.997 | 43.290 | 63.969 | 1.00 | 26.07  |
| ATOM | 582 | N   | GLU | A | 77 | -15.973 | 42.281 | 65.736 | 1.00 | 32.78  |
| ATOM | 583 | CA  | GLU | A | 77 | -15.539 | 43.318 | 66.645 | 1.00 | 34.78  |
| ATOM | 584 | C   | GLU | A | 77 | -14.050 | 43.214 | 66.886 | 1.00 | 38.63  |
| ATOM | 585 | O   | GLU | A | 77 | -13.431 | 42.176 | 66.641 | 1.00 | 34.85  |
| ATOM | 586 | CB  | GLU | A | 77 | -16.337 | 43.338 | 67.966 | 1.00 | 37.18  |
| ATOM | 587 | CG  | GLU | A | 77 | -16.506 | 41.956 | 68.643 | 1.00 | 56.65  |
| ATOM | 588 | CD  | GLU | A | 77 | -16.316 | 41.990 | 70.151 | 1.00 | 100.00 |
| ATOM | 589 | OE1 | GLU | A | 77 | -16.789 | 42.859 | 70.877 | 1.00 | 100.00 |
| ATOM | 590 | OE2 | GLU | A | 77 | -15.603 | 40.975 | 70.597 | 1.00 | 100.00 |
| ATOM | 591 | N   | ARG | A | 78 | -13.483 | 44.312 | 67.343 | 1.00 | 37.73  |
| ATOM | 592 | CA  | ARG | A | 78 | -12.068 | 44.336 | 67.624 | 1.00 | 37.11  |
| ATOM | 593 | C   | ARG | A | 78 | -11.709 | 43.545 | 68.889 | 1.00 | 39.61  |
| ATOM | 594 | O   | ARG | A | 78 | -12.422 | 43.549 | 69.906 | 1.00 | 36.40  |
| ATOM | 595 | CB  | ARG | A | 78 | -11.522 | 45.744 | 67.693 | 1.00 | 33.62  |
| ATOM | 596 | CG  | ARG | A | 78 | -9.991  | 45.807 | 67.699 | 1.00 | 34.93  |
| ATOM | 597 | CD  | ARG | A | 78 | -9.516  | 47.207 | 68.040 | 1.00 | 32.03  |
| ATOM | 598 | NE  | ARG | A | 78 | -8.083  | 47.397 | 68.058 | 1.00 | 33.71  |
| ATOM | 599 | CZ  | ARG | A | 78 | -7.459  | 48.239 | 67.241 | 1.00 | 53.03  |
| ATOM | 600 | NH1 | ARG | A | 78 | -8.114  | 48.941 | 66.314 | 1.00 | 39.56  |
| ATOM | 601 | NH2 | ARG | A | 78 | -6.139  | 48.361 | 67.337 | 1.00 | 53.05  |
| ATOM | 602 | N   | GLN | A | 79 | -10.576 | 42.842 | 68.795 | 1.00 | 33.34  |
| ATOM | 603 | CA  | GLN | A | 79 | -10.044 | 42.052 | 69.881 | 1.00 | 32.25  |
| ATOM | 604 | C   | GLN | A | 79 | -8.708  | 42.662 | 70.221 | 1.00 | 36.49  |
| ATOM | 605 | O   | GLN | A | 79 | -7.651  | 42.164 | 69.834 | 1.00 | 37.41  |
| ATOM | 606 | CB  | GLN | A | 79 | -9.906  | 40.580 | 69.472 | 1.00 | 31.80  |
| ATOM | 607 | CG  | GLN | A | 79 | -11.263 | 39.972 | 69.092 | 1.00 | 31.70  |
| ATOM | 608 | CD  | GLN | A | 79 | -11.143 | 38.511 | 68.713 | 1.00 | 62.24  |
| ATOM | 609 | OE1 | GLN | A | 79 | -10.234 | 37.819 | 69.182 | 1.00 | 64.13  |
| ATOM | 610 | NE2 | GLN | A | 79 | -12.046 | 38.033 | 67.862 | 1.00 | 56.77  |
| ATOM | 611 | N   | SER | A | 80 | -8.787  | 43.794 | 70.893 | 1.00 | 30.40  |
| ATOM | 612 | CA  | SER | A | 80 | -7.617  | 44.551 | 71.284 | 1.00 | 27.48  |
| ATOM | 613 | C   | SER | A | 80 | -6.535  | 44.592 | 70.257 | 1.00 | 29.91  |
| ATOM | 614 | O   | SER | A | 80 | -6.758  | 45.054 | 69.140 | 1.00 | 28.75  |
| ATOM | 615 | CB  | SER | A | 80 | -7.066  | 44.252 | 72.655 | 1.00 | 27.52  |
| ATOM | 616 | OG  | SER | A | 80 | -7.173  | 42.874 | 72.863 | 1.00 | 44.76  |
| ATOM | 617 | N   | TYR | A | 81 | -5.350  | 44.133 | 70.671 | 1.00 | 27.38  |
| ATOM | 618 | CA  | TYR | A | 81 | -4.162  | 44.180 | 69.820 | 1.00 | 25.29  |
| ATOM | 619 | C   | TYR | A | 81 | -4.196  | 43.286 | 68.604 | 1.00 | 23.60  |
| ATOM | 620 | O   | TYR | A | 81 | -3.389  | 43.435 | 67.710 | 1.00 | 26.12  |
| ATOM | 621 | CB  | TYR | A | 81 | -2.861  | 43.992 | 70.632 | 1.00 | 23.78  |
| ATOM | 622 | CG  | TYR | A | 81 | -2.849  | 42.621 | 71.190 | 1.00 | 21.01  |
| ATOM | 623 | CD1 | TYR | A | 81 | -3.374  | 42.361 | 72.450 | 1.00 | 20.45  |
| ATOM | 624 | CD2 | TYR | A | 81 | -2.387  | 41.569 | 70.406 | 1.00 | 23.13  |
| ATOM | 625 | CE1 | TYR | A | 81 | -3.402  | 41.064 | 72.948 | 1.00 | 18.45  |
| ATOM | 626 | CE2 | TYR | A | 81 | -2.426  | 40.263 | 70.885 | 1.00 | 24.91  |
| ATOM | 627 | CZ  | TYR | A | 81 | -2.929  | 40.017 | 72.162 | 1.00 | 26.97  |
| ATOM | 628 | OH  | TYR | A | 81 | -2.960  | 38.731 | 72.652 | 1.00 | 35.08  |
| ATOM | 629 | N   | LYS | A | 82 | -5.125  | 42.370 | 68.568 | 1.00 | 19.77  |
| ATOM | 630 | CA  | LYS | A | 82 | -5.225  | 41.448 | 67.433 | 1.00 | 19.65  |
| ATOM | 631 | C   | LYS | A | 82 | -5.948  | 42.036 | 66.232 | 1.00 | 26.75  |
| ATOM | 632 | O   | LYS | A | 82 | -5.821  | 41.545 | 65.107 | 1.00 | 26.09  |



|      |     |     |     |   |    |         |        |        |      |       |
|------|-----|-----|-----|---|----|---------|--------|--------|------|-------|
| ATOM | 633 | CB  | LYS | A | 82 | -5.929  | 40.217 | 67.888 | 1.00 | 19.96 |
| ATOM | 634 | CG  | LYS | A | 82 | -5.039  | 39.427 | 68.808 | 1.00 | 39.72 |
| ATOM | 635 | CD  | LYS | A | 82 | -5.610  | 38.058 | 69.103 | 1.00 | 45.35 |
| ATOM | 636 | CE  | LYS | A | 82 | -5.868  | 37.809 | 70.577 | 1.00 | 52.66 |
| ATOM | 637 | NZ  | LYS | A | 82 | -6.016  | 36.375 | 70.879 | 1.00 | 51.38 |
| ATOM | 638 | N   | GLY | A | 83 | -6.698  | 43.114 | 66.482 | 1.00 | 25.62 |
| ATOM | 639 | CA  | GLY | A | 83 | -7.465  | 43.786 | 65.441 | 1.00 | 24.64 |
| ATOM | 640 | C   | GLY | A | 83 | -8.857  | 43.145 | 65.324 | 1.00 | 26.15 |
| ATOM | 641 | O   | GLY | A | 83 | -9.348  | 42.515 | 66.255 | 1.00 | 24.12 |
| ATOM | 642 | N   | SER | A | 84 | -9.463  | 43.273 | 64.136 | 1.00 | 27.22 |
| ATOM | 643 | CA  | SER | A | 84 | -10.806 | 42.770 | 63.829 | 1.00 | 27.17 |
| ATOM | 644 | C   | SER | A | 84 | -10.815 | 41.744 | 62.720 | 1.00 | 29.72 |
| ATOM | 645 | O   | SER | A | 84 | -10.237 | 41.933 | 61.649 | 1.00 | 30.39 |
| ATOM | 646 | CB  | SER | A | 84 | -11.708 | 43.929 | 63.377 | 1.00 | 31.94 |
| ATOM | 647 | OG  | SER | A | 84 | -11.719 | 44.976 | 64.344 | 1.00 | 42.05 |
| ATOM | 648 | N   | PRO | A | 85 | -11.513 | 40.667 | 62.979 | 1.00 | 24.61 |
| ATOM | 649 | CA  | PRO | A | 85 | -11.640 | 39.590 | 62.017 | 1.00 | 25.06 |
| ATOM | 650 | C   | PRO | A | 85 | -12.480 | 40.005 | 60.819 | 1.00 | 33.19 |
| ATOM | 651 | O   | PRO | A | 85 | -13.536 | 40.622 | 60.995 | 1.00 | 31.19 |
| ATOM | 652 | CB  | PRO | A | 85 | -12.404 | 38.469 | 62.736 | 1.00 | 24.61 |
| ATOM | 653 | CG  | PRO | A | 85 | -12.959 | 39.049 | 64.014 | 1.00 | 30.62 |
| ATOM | 654 | CD  | PRO | A | 85 | -12.314 | 40.423 | 64.199 | 1.00 | 26.23 |
| ATOM | 655 | N   | MET | A | 86 | -12.019 | 39.632 | 59.623 | 1.00 | 28.27 |
| ATOM | 656 | CA  | MET | A | 86 | -12.754 | 39.924 | 58.411 | 1.00 | 27.27 |
| ATOM | 657 | C   | MET | A | 86 | -13.227 | 38.650 | 57.699 | 1.00 | 32.93 |
| ATOM | 658 | O   | MET | A | 86 | -12.438 | 37.997 | 57.038 | 1.00 | 27.77 |
| ATOM | 659 | CB  | MET | A | 86 | -11.930 | 40.743 | 57.451 | 1.00 | 27.52 |
| ATOM | 660 | CG  | MET | A | 86 | -12.756 | 41.222 | 56.274 | 1.00 | 30.43 |
| ATOM | 661 | SD  | MET | A | 86 | -11.679 | 41.978 | 55.050 | 1.00 | 37.30 |
| ATOM | 662 | CE  | MET | A | 86 | -12.815 | 42.248 | 53.681 | 1.00 | 37.61 |
| ATOM | 663 | N   | GLU | A | 87 | -14.507 | 38.295 | 57.832 | 1.00 | 34.14 |
| ATOM | 664 | CA  | GLU | A | 87 | -15.060 | 37.093 | 57.184 | 1.00 | 36.06 |
| ATOM | 665 | C   | GLU | A | 87 | -15.538 | 37.367 | 55.766 | 1.00 | 39.45 |
| ATOM | 666 | O   | GLU | A | 87 | -16.366 | 38.250 | 55.586 | 1.00 | 41.63 |
| ATOM | 667 | CB  | GLU | A | 87 | -16.211 | 36.499 | 58.003 | 1.00 | 37.41 |
| ATOM | 668 | CG  | GLU | A | 87 | -16.540 | 35.036 | 57.655 | 1.00 | 43.37 |
| ATOM | 669 | CD  | GLU | A | 87 | -17.445 | 34.371 | 58.657 | 1.00 | 60.02 |
| ATOM | 670 | OE1 | GLU | A | 87 | -18.629 | 34.637 | 58.785 | 1.00 | 83.59 |
| ATOM | 671 | OE2 | GLU | A | 87 | -16.827 | 33.467 | 59.375 | 1.00 | 74.01 |
| ATOM | 672 | N   | ILE | A | 88 | -15.000 | 36.608 | 54.788 | 1.00 | 34.85 |
| ATOM | 673 | CA  | ILE | A | 88 | -15.343 | 36.698 | 53.359 | 1.00 | 33.18 |
| ATOM | 674 | C   | ILE | A | 88 | -16.170 | 35.489 | 52.896 | 1.00 | 42.28 |
| ATOM | 675 | O   | ILE | A | 88 | -15.895 | 34.352 | 53.254 | 1.00 | 43.61 |
| ATOM | 676 | CB  | ILE | A | 88 | -14.122 | 36.878 | 52.475 | 1.00 | 33.03 |
| ATOM | 677 | CG1 | ILE | A | 88 | -13.251 | 38.003 | 53.020 | 1.00 | 31.03 |
| ATOM | 678 | CG2 | ILE | A | 88 | -14.525 | 37.171 | 51.035 | 1.00 | 31.15 |
| ATOM | 679 | CD1 | ILE | A | 88 | -12.088 | 38.331 | 52.096 | 1.00 | 33.21 |
| ATOM | 680 | N   | SER | A | 89 | -17.222 | 35.723 | 52.116 | 1.00 | 41.90 |
| ATOM | 681 | CA  | SER | A | 89 | -18.072 | 34.635 | 51.633 | 1.00 | 40.20 |
| ATOM | 682 | C   | SER | A | 89 | -17.689 | 34.229 | 50.234 | 1.00 | 43.89 |
| ATOM | 683 | O   | SER | A | 89 | -17.731 | 35.037 | 49.296 | 1.00 | 40.79 |
| ATOM | 684 | CB  | SER | A | 89 | -19.557 | 34.959 | 51.685 | 1.00 | 43.23 |
| ATOM | 685 | OG  | SER | A | 89 | -20.042 | 34.675 | 52.986 | 1.00 | 57.92 |
| ATOM | 686 | N   | LEU | A | 90 | -17.298 | 32.967 | 50.099 | 1.00 | 41.94 |
| ATOM | 687 | CA  | LEU | A | 90 | -16.945 | 32.481 | 48.793 | 1.00 | 41.32 |
| ATOM | 688 | C   | LEU | A | 90 | -18.258 | 32.175 | 48.106 | 1.00 | 41.86 |
| ATOM | 689 | O   | LEU | A | 90 | -19.186 | 31.608 | 48.692 | 1.00 | 41.35 |
| ATOM | 690 | CB  | LEU | A | 90 | -16.014 | 31.252 | 48.856 | 1.00 | 41.25 |



|      |     |     |     |   |    |         |        |        |      |        |
|------|-----|-----|-----|---|----|---------|--------|--------|------|--------|
| ATOM | 691 | CG  | LEU | A | 90 | -14.827 | 31.484 | 49.781 | 1.00 | 43.31  |
| ATOM | 692 | CD1 | LEU | A | 90 | -14.050 | 30.182 | 50.020 | 1.00 | 40.39  |
| ATOM | 693 | CD2 | LEU | A | 90 | -13.940 | 32.569 | 49.162 | 1.00 | 40.88  |
| ATOM | 694 | N   | PRO | A | 91 | -18.337 | 32.612 | 46.887 | 1.00 | 40.52  |
| ATOM | 695 | CA  | PRO | A | 91 | -19.516 | 32.434 | 46.056 | 1.00 | 43.11  |
| ATOM | 696 | C   | PRO | A | 91 | -19.516 | 31.058 | 45.401 | 1.00 | 51.36  |
| ATOM | 697 | O   | PRO | A | 91 | -20.363 | 30.753 | 44.576 | 1.00 | 52.06  |
| ATOM | 698 | CB  | PRO | A | 91 | -19.359 | 33.470 | 44.942 | 1.00 | 43.83  |
| ATOM | 699 | CG  | PRO | A | 91 | -17.883 | 33.867 | 44.915 | 1.00 | 48.09  |
| ATOM | 700 | CD  | PRO | A | 91 | -17.268 | 33.373 | 46.217 | 1.00 | 41.44  |
| ATOM | 701 | N   | ILE | A | 92 | -18.516 | 30.261 | 45.767 | 1.00 | 50.02  |
| ATOM | 702 | CA  | ILE | A | 92 | -18.325 | 28.924 | 45.259 | 1.00 | 50.50  |
| ATOM | 703 | C   | ILE | A | 92 | -17.525 | 28.128 | 46.242 | 1.00 | 47.69  |
| ATOM | 704 | O   | ILE | A | 92 | -16.416 | 28.497 | 46.564 | 1.00 | 46.80  |
| ATOM | 705 | CB  | ILE | A | 92 | -17.492 | 28.924 | 44.001 | 1.00 | 55.84  |
| ATOM | 706 | CG1 | ILE | A | 92 | -18.372 | 29.135 | 42.791 | 1.00 | 58.16  |
| ATOM | 707 | CG2 | ILE | A | 92 | -16.776 | 27.584 | 43.884 | 1.00 | 59.08  |
| ATOM | 708 | CD1 | ILE | A | 92 | -17.568 | 29.038 | 41.493 | 1.00 | 83.51  |
| ATOM | 709 | N   | ALA | A | 93 | -18.047 | 27.023 | 46.683 | 1.00 | 40.78  |
| ATOM | 710 | CA  | ALA | A | 93 | -17.280 | 26.257 | 47.599 | 1.00 | 38.66  |
| ATOM | 711 | C   | ALA | A | 93 | -16.066 | 25.735 | 46.892 | 1.00 | 45.36  |
| ATOM | 712 | O   | ALA | A | 93 | -16.141 | 25.391 | 45.720 | 1.00 | 47.87  |
| ATOM | 713 | CB  | ALA | A | 93 | -18.114 | 25.149 | 48.205 | 1.00 | 38.35  |
| ATOM | 714 | N   | LEU | A | 94 | -14.956 | 25.716 | 47.630 | 1.00 | 42.52  |
| ATOM | 715 | CA  | LEU | A | 94 | -13.652 | 25.233 | 47.181 | 1.00 | 41.33  |
| ATOM | 716 | C   | LEU | A | 94 | -13.330 | 23.900 | 47.814 | 1.00 | 46.96  |
| ATOM | 717 | O   | LEU | A | 94 | -13.719 | 23.618 | 48.948 | 1.00 | 45.93  |
| ATOM | 718 | CB  | LEU | A | 94 | -12.515 | 26.182 | 47.571 | 1.00 | 39.52  |
| ATOM | 719 | CG  | LEU | A | 94 | -12.515 | 27.449 | 46.748 | 1.00 | 44.05  |
| ATOM | 720 | CD1 | LEU | A | 94 | -11.153 | 28.133 | 46.829 | 1.00 | 44.88  |
| ATOM | 721 | CD2 | LEU | A | 94 | -12.843 | 27.115 | 45.305 | 1.00 | 45.42  |
| ATOM | 722 | N   | SER | A | 95 | -12.604 | 23.083 | 47.074 | 1.00 | 44.42  |
| ATOM | 723 | CA  | SER | A | 95 | -12.221 | 21.807 | 47.591 | 1.00 | 43.44  |
| ATOM | 724 | C   | SER | A | 95 | -10.728 | 21.776 | 47.719 | 1.00 | 36.96  |
| ATOM | 725 | O   | SER | A | 95 | -10.038 | 22.639 | 47.187 | 1.00 | 33.14  |
| ATOM | 726 | CB  | SER | A | 95 | -12.739 | 20.704 | 46.696 | 1.00 | 51.13  |
| ATOM | 727 | OG  | SER | A | 95 | -14.083 | 20.459 | 47.074 | 1.00 | 60.97  |
| ATOM | 728 | N   | LYS | A | 96 | -10.240 | 20.779 | 48.407 | 1.00 | 33.03  |
| ATOM | 729 | CA  | LYS | A | 96 | -8.818  | 20.694 | 48.557 | 1.00 | 33.15  |
| ATOM | 730 | C   | LYS | A | 96 | -8.122  | 21.204 | 47.321 | 1.00 | 37.16  |
| ATOM | 731 | O   | LYS | A | 96 | -8.514  | 20.922 | 46.188 | 1.00 | 38.12  |
| ATOM | 732 | CB  | LYS | A | 96 | -8.348  | 19.290 | 48.861 | 1.00 | 34.42  |
| ATOM | 733 | CG  | LYS | A | 96 | -8.583  | 18.910 | 50.298 | 1.00 | 57.96  |
| ATOM | 734 | CD  | LYS | A | 96 | -8.422  | 17.423 | 50.553 | 1.00 | 73.54  |
| ATOM | 735 | CE  | LYS | A | 96 | -9.475  | 16.882 | 51.512 | 1.00 | 94.46  |
| ATOM | 736 | NZ  | LYS | A | 96 | -9.837  | 15.475 | 51.246 | 1.00 | 100.00 |
| ATOM | 737 | N   | ASN | A | 97 | -7.069  | 21.958 | 47.573 | 1.00 | 29.05  |
| ATOM | 738 | CA  | ASN | A | 97 | -6.213  | 22.528 | 46.568 | 1.00 | 25.85  |
| ATOM | 739 | C   | ASN | A | 97 | -6.783  | 23.479 | 45.576 | 1.00 | 31.84  |
| ATOM | 740 | O   | ASN | A | 97 | -6.064  | 23.909 | 44.682 | 1.00 | 33.02  |
| ATOM | 741 | CB  | ASN | A | 97 | -5.166  | 21.572 | 46.006 | 1.00 | 33.23  |
| ATOM | 742 | CG  | ASN | A | 97 | -4.289  | 21.018 | 47.135 | 1.00 | 55.19  |
| ATOM | 743 | OD1 | ASN | A | 97 | -4.009  | 19.823 | 47.186 | 1.00 | 56.15  |
| ATOM | 744 | ND2 | ASN | A | 97 | -3.873  | 21.867 | 48.073 | 1.00 | 43.36  |
| ATOM | 745 | N   | GLN | A | 98 | -8.053  | 23.835 | 45.730 | 1.00 | 32.99  |
| ATOM | 746 | CA  | GLN | A | 98 | -8.611  | 24.798 | 44.792 | 1.00 | 35.56  |
| ATOM | 747 | C   | GLN | A | 98 | -8.259  | 26.220 | 45.204 | 1.00 | 40.34  |
| ATOM | 748 | O   | GLN | A | 98 | -8.208  | 26.541 | 46.381 | 1.00 | 37.21  |



|      |     |     |     |   |     |         |        |        |      |        |
|------|-----|-----|-----|---|-----|---------|--------|--------|------|--------|
| ATOM | 749 | CB  | GLN | A | 98  | -10.111 | 24.610 | 44.555 | 1.00 | 38.17  |
| ATOM | 750 | CG  | GLN | A | 98  | -10.446 | 23.220 | 43.974 | 1.00 | 47.37  |
| ATOM | 751 | CD  | GLN | A | 98  | -11.869 | 23.144 | 43.480 | 1.00 | 68.06  |
| ATOM | 752 | OE1 | GLN | A | 98  | -12.676 | 22.343 | 43.981 | 1.00 | 68.25  |
| ATOM | 753 | NE2 | GLN | A | 98  | -12.184 | 24.014 | 42.527 | 1.00 | 58.46  |
| ATOM | 754 | N   | GLU | A | 99  | -8.007  | 27.049 | 44.206 | 1.00 | 42.57  |
| ATOM | 755 | CA  | GLU | A | 99  | -7.630  | 28.442 | 44.380 | 1.00 | 43.65  |
| ATOM | 756 | C   | GLU | A | 99  | -8.649  | 29.427 | 43.778 | 1.00 | 47.15  |
| ATOM | 757 | O   | GLU | A | 99  | -9.262  | 29.166 | 42.734 | 1.00 | 44.38  |
| ATOM | 758 | CB  | GLU | A | 99  | -6.229  | 28.688 | 43.745 | 1.00 | 44.65  |
| ATOM | 759 | CG  | GLU | A | 99  | -5.210  | 27.549 | 44.026 | 1.00 | 62.98  |
| ATOM | 760 | CD  | GLU | A | 99  | -3.804  | 27.766 | 43.496 | 1.00 | 92.15  |
| ATOM | 761 | OE1 | GLU | A | 99  | -3.299  | 28.867 | 43.338 | 1.00 | 100.00 |
| ATOM | 762 | OE2 | GLU | A | 99  | -3.191  | 26.625 | 43.252 | 1.00 | 78.70  |
| ATOM | 763 | N   | ILE | A | 100 | -8.801  | 30.565 | 44.468 | 1.00 | 41.83  |
| ATOM | 764 | CA  | ILE | A | 100 | -9.632  | 31.698 | 44.080 | 1.00 | 38.88  |
| ATOM | 765 | C   | ILE | A | 100 | -8.784  | 32.895 | 44.373 | 1.00 | 43.54  |
| ATOM | 766 | O   | ILE | A | 100 | -7.812  | 32.830 | 45.135 | 1.00 | 42.91  |
| ATOM | 767 | CB  | ILE | A | 100 | -10.879 | 31.971 | 44.904 | 1.00 | 42.18  |
| ATOM | 768 | CG1 | ILE | A | 100 | -10.849 | 31.355 | 46.271 | 1.00 | 47.13  |
| ATOM | 769 | CG2 | ILE | A | 100 | -12.225 | 31.875 | 44.204 | 1.00 | 41.40  |
| ATOM | 770 | CD1 | ILE | A | 100 | -10.493 | 32.395 | 47.331 | 1.00 | 74.72  |
| ATOM | 771 | N   | VAL | A | 101 | -9.156  | 34.001 | 43.784 | 1.00 | 39.29  |
| ATOM | 772 | CA  | VAL | A | 101 | -8.461  | 35.229 | 44.067 | 1.00 | 37.27  |
| ATOM | 773 | C   | VAL | A | 101 | -9.435  | 36.255 | 44.626 | 1.00 | 39.62  |
| ATOM | 774 | O   | VAL | A | 101 | -10.516 | 36.464 | 44.098 | 1.00 | 38.28  |
| ATOM | 775 | CB  | VAL | A | 101 | -7.425  | 35.723 | 43.080 | 1.00 | 36.91  |
| ATOM | 776 | CG1 | VAL | A | 101 | -7.497  | 34.980 | 41.770 | 1.00 | 34.64  |
| ATOM | 777 | CG2 | VAL | A | 101 | -7.482  | 37.237 | 42.939 | 1.00 | 35.34  |
| ATOM | 778 | N   | ILE | A | 102 | -9.078  | 36.828 | 45.749 | 1.00 | 31.68  |
| ATOM | 779 | CA  | ILE | A | 102 | -9.924  | 37.777 | 46.403 | 1.00 | 28.22  |
| ATOM | 780 | C   | ILE | A | 102 | -9.328  | 39.135 | 46.284 | 1.00 | 31.14  |
| ATOM | 781 | O   | ILE | A | 102 | -8.173  | 39.344 | 46.618 | 1.00 | 31.20  |
| ATOM | 782 | CB  | ILE | A | 102 | -10.086 | 37.348 | 47.841 | 1.00 | 30.22  |
| ATOM | 783 | CG1 | ILE | A | 102 | -10.432 | 35.863 | 47.821 | 1.00 | 30.27  |
| ATOM | 784 | CG2 | ILE | A | 102 | -11.214 | 38.112 | 48.495 | 1.00 | 30.53  |
| ATOM | 785 | CD1 | ILE | A | 102 | -10.807 | 35.275 | 49.187 | 1.00 | 36.83  |
| ATOM | 786 | N   | GLU | A | 103 | -10.087 | 40.073 | 45.761 | 1.00 | 26.48  |
| ATOM | 787 | CA  | GLU | A | 103 | -9.510  | 41.390 | 45.655 | 1.00 | 30.38  |
| ATOM | 788 | C   | GLU | A | 103 | -10.196 | 42.340 | 46.596 | 1.00 | 38.06  |
| ATOM | 789 | O   | GLU | A | 103 | -11.400 | 42.583 | 46.488 | 1.00 | 39.31  |
| ATOM | 790 | CB  | GLU | A | 103 | -9.496  | 41.944 | 44.256 | 1.00 | 31.96  |
| ATOM | 791 | CG  | GLU | A | 103 | -9.063  | 43.403 | 44.237 | 1.00 | 41.76  |
| ATOM | 792 | CD  | GLU | A | 103 | -9.594  | 44.045 | 43.003 | 1.00 | 80.28  |
| ATOM | 793 | OE1 | GLU | A | 103 | -10.653 | 44.658 | 42.976 | 1.00 | 97.93  |
| ATOM | 794 | OE2 | GLU | A | 103 | -8.842  | 43.798 | 41.957 | 1.00 | 70.69  |
| ATOM | 795 | N   | ILE | A | 104 | -9.409  | 42.831 | 47.536 | 1.00 | 33.55  |
| ATOM | 796 | CA  | ILE | A | 104 | -9.900  | 43.716 | 48.562 | 1.00 | 30.57  |
| ATOM | 797 | C   | ILE | A | 104 | -9.417  | 45.121 | 48.376 | 1.00 | 32.37  |
| ATOM | 798 | O   | ILE | A | 104 | -8.209  | 45.395 | 48.262 | 1.00 | 28.32  |
| ATOM | 799 | CB  | ILE | A | 104 | -9.522  | 43.227 | 49.955 | 1.00 | 33.68  |
| ATOM | 800 | CG1 | ILE | A | 104 | -9.880  | 41.763 | 50.117 | 1.00 | 31.76  |
| ATOM | 801 | CG2 | ILE | A | 104 | -10.221 | 44.054 | 51.024 | 1.00 | 32.15  |
| ATOM | 802 | CD1 | ILE | A | 104 | -9.097  | 41.073 | 51.227 | 1.00 | 34.97  |
| ATOM | 803 | N   | SER | A | 105 | -10.433 | 45.980 | 48.336 | 1.00 | 35.99  |
| ATOM | 804 | CA  | SER | A | 105 | -10.304 | 47.420 | 48.202 | 1.00 | 37.06  |
| ATOM | 805 | C   | SER | A | 105 | -10.231 | 47.965 | 49.624 | 1.00 | 32.66  |
| ATOM | 806 | O   | SER | A | 105 | -11.184 | 47.854 | 50.409 | 1.00 | 27.10  |



66920:07F09

|      |     |     |     |   |     |         |        |        |      |        |
|------|-----|-----|-----|---|-----|---------|--------|--------|------|--------|
| ATOM | 807 | CB  | SER | A | 105 | -11.479 | 48.007 | 47.438 | 1.00 | 41.57  |
| ATOM | 808 | OG  | SER | A | 105 | -11.142 | 48.056 | 46.066 | 1.00 | 42.85  |
| ATOM | 809 | N   | PHE | A | 106 | -9.069  | 48.495 | 49.970 | 1.00 | 26.79  |
| ATOM | 810 | CA  | PHE | A | 106 | -8.932  | 48.950 | 51.316 | 1.00 | 24.44  |
| ATOM | 811 | C   | PHE | A | 106 | -8.247  | 50.298 | 51.442 | 1.00 | 27.41  |
| ATOM | 812 | O   | PHE | A | 106 | -7.592  | 50.835 | 50.512 | 1.00 | 23.66  |
| ATOM | 813 | CB  | PHE | A | 106 | -8.098  | 47.870 | 52.069 | 1.00 | 25.82  |
| ATOM | 814 | CG  | PHE | A | 106 | -6.659  | 47.899 | 51.602 | 1.00 | 26.84  |
| ATOM | 815 | CD1 | PHE | A | 106 | -6.279  | 47.176 | 50.473 | 1.00 | 29.09  |
| ATOM | 816 | CD2 | PHE | A | 106 | -5.690  | 48.683 | 52.244 | 1.00 | 26.96  |
| ATOM | 817 | CE1 | PHE | A | 106 | -4.959  | 47.223 | 50.019 | 1.00 | 30.72  |
| ATOM | 818 | CE2 | PHE | A | 106 | -4.371  | 48.760 | 51.788 | 1.00 | 27.84  |
| ATOM | 819 | CZ  | PHE | A | 106 | -4.003  | 48.008 | 50.670 | 1.00 | 27.74  |
| ATOM | 820 | N   | GLU | A | 107 | -8.390  | 50.814 | 52.669 | 1.00 | 27.81  |
| ATOM | 821 | CA  | GLU | A | 107 | -7.776  | 52.082 | 53.054 | 1.00 | 30.68  |
| ATOM | 822 | C   | GLU | A | 107 | -7.255  | 52.010 | 54.493 | 1.00 | 30.66  |
| ATOM | 823 | O   | GLU | A | 107 | -7.991  | 51.628 | 55.409 | 1.00 | 32.52  |
| ATOM | 824 | CB  | GLU | A | 107 | -8.744  | 53.268 | 52.866 | 1.00 | 33.19  |
| ATOM | 825 | CG  | GLU | A | 107 | -8.059  | 54.652 | 52.795 | 1.00 | 50.92  |
| ATOM | 826 | CD  | GLU | A | 107 | -9.053  | 55.794 | 52.621 | 1.00 | 75.89  |
| ATOM | 827 | OE1 | GLU | A | 107 | -9.430  | 56.225 | 51.535 | 1.00 | 61.91  |
| ATOM | 828 | OE2 | GLU | A | 107 | -9.483  | 56.292 | 53.762 | 1.00 | 47.17  |
| ATOM | 829 | N   | THR | A | 108 | -5.978  | 52.366 | 54.682 | 1.00 | 26.11  |
| ATOM | 830 | CA  | THR | A | 108 | -5.341  | 52.325 | 56.009 | 1.00 | 28.04  |
| ATOM | 831 | C   | THR | A | 108 | -5.664  | 53.563 | 56.790 | 1.00 | 32.96  |
| ATOM | 832 | O   | THR | A | 108 | -5.881  | 54.618 | 56.202 | 1.00 | 30.16  |
| ATOM | 833 | CB  | THR | A | 108 | -3.787  | 52.277 | 55.957 | 1.00 | 35.08  |
| ATOM | 834 | OG1 | THR | A | 108 | -3.245  | 53.465 | 55.378 | 1.00 | 29.19  |
| ATOM | 835 | CG2 | THR | A | 108 | -3.254  | 51.032 | 55.245 | 1.00 | 32.38  |
| ATOM | 836 | N   | SER | A | 109 | -5.650  | 53.417 | 58.112 | 1.00 | 28.09  |
| ATOM | 837 | CA  | SER | A | 109 | -5.890  | 54.508 | 59.057 | 1.00 | 22.39  |
| ATOM | 838 | C   | SER | A | 109 | -4.612  | 55.300 | 59.248 | 1.00 | 26.59  |
| ATOM | 839 | O   | SER | A | 109 | -3.497  | 54.766 | 59.191 | 1.00 | 23.06  |
| ATOM | 840 | CB  | SER | A | 109 | -6.316  | 53.896 | 60.386 | 1.00 | 23.90  |
| ATOM | 841 | OG  | SER | A | 109 | -6.087  | 54.804 | 61.448 | 1.00 | 27.48  |
| ATOM | 842 | N   | PRO | A | 110 | -4.720  | 56.594 | 59.495 | 1.00 | 28.89  |
| ATOM | 843 | CA  | PRO | A | 110 | -3.481  | 57.312 | 59.703 | 1.00 | 27.31  |
| ATOM | 844 | C   | PRO | A | 110 | -2.840  | 56.838 | 60.993 | 1.00 | 27.91  |
| ATOM | 845 | O   | PRO | A | 110 | -1.651  | 57.033 | 61.172 | 1.00 | 28.30  |
| ATOM | 846 | CB  | PRO | A | 110 | -3.776  | 58.792 | 59.689 | 1.00 | 28.41  |
| ATOM | 847 | CG  | PRO | A | 110 | -5.188  | 58.921 | 59.138 | 1.00 | 33.97  |
| ATOM | 848 | CD  | PRO | A | 110 | -5.820  | 57.545 | 59.214 | 1.00 | 30.89  |
| ATOM | 849 | N   | LYS | A | 111 | -3.640  | 56.170 | 61.848 | 1.00 | 21.21  |
| ATOM | 850 | CA  | LYS | A | 111 | -3.137  | 55.620 | 63.098 | 1.00 | 21.20  |
| ATOM | 851 | C   | LYS | A | 111 | -2.634  | 54.163 | 62.972 | 1.00 | 24.12  |
| ATOM | 852 | O   | LYS | A | 111 | -2.502  | 53.476 | 63.990 | 1.00 | 27.31  |
| ATOM | 853 | CB  | LYS | A | 111 | -4.188  | 55.688 | 64.202 | 1.00 | 24.13  |
| ATOM | 854 | CG  | LYS | A | 111 | -4.435  | 57.079 | 64.786 | 1.00 | 44.09  |
| ATOM | 855 | CD  | LYS | A | 111 | -5.146  | 58.027 | 63.832 | 1.00 | 80.95  |
| ATOM | 856 | CE  | LYS | A | 111 | -6.627  | 57.733 | 63.614 | 1.00 | 100.00 |
| ATOM | 857 | NZ  | LYS | A | 111 | -7.193  | 58.483 | 62.473 | 1.00 | 100.00 |
| ATOM | 858 | N   | SER | A | 112 | -2.371  | 53.669 | 61.743 | 1.00 | 21.95  |
| ATOM | 859 | CA  | SER | A | 112 | -1.891  | 52.278 | 61.499 | 1.00 | 21.09  |
| ATOM | 860 | C   | SER | A | 112 | -0.709  | 51.968 | 62.438 | 1.00 | 23.23  |
| ATOM | 861 | O   | SER | A | 112 | 0.236   | 52.722 | 62.472 | 1.00 | 25.25  |
| ATOM | 862 | CB  | SER | A | 112 | -1.467  | 52.084 | 60.034 | 1.00 | 17.80  |
| ATOM | 863 | OG  | SER | A | 112 | -0.821  | 50.850 | 59.845 | 1.00 | 19.72  |
| ATOM | 864 | N   | SER | A | 113 | -0.752  | 50.884 | 63.203 | 1.00 | 19.64  |



|      |     |     |     |   |     |        |        |        |      |       |
|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 865 | CA  | SER | A | 113 | 0.342  | 50.587 | 64.087 | 1.00 | 16.68 |
| ATOM | 866 | C   | SER | A | 113 | 1.539  | 50.087 | 63.316 | 1.00 | 22.16 |
| ATOM | 867 | O   | SER | A | 113 | 2.653  | 50.005 | 63.822 | 1.00 | 21.53 |
| ATOM | 868 | CB  | SER | A | 113 | -0.061 | 49.633 | 65.183 | 1.00 | 20.15 |
| ATOM | 869 | OG  | SER | A | 113 | -0.358 | 48.369 | 64.663 | 1.00 | 23.41 |
| ATOM | 870 | N   | ALA | A | 114 | 1.325  | 49.741 | 62.059 | 1.00 | 21.04 |
| ATOM | 871 | CA  | ALA | A | 114 | 2.432  | 49.266 | 61.221 | 1.00 | 19.34 |
| ATOM | 872 | C   | ALA | A | 114 | 3.212  | 50.412 | 60.581 | 1.00 | 20.25 |
| ATOM | 873 | O   | ALA | A | 114 | 4.287  | 50.210 | 60.004 | 1.00 | 20.84 |
| ATOM | 874 | CB  | ALA | A | 114 | 1.876  | 48.455 | 60.061 | 1.00 | 19.26 |
| ATOM | 875 | N   | LEU | A | 115 | 2.636  | 51.614 | 60.636 | 1.00 | 17.27 |
| ATOM | 876 | CA  | LEU | A | 115 | 3.281  | 52.725 | 59.992 | 1.00 | 19.18 |
| ATOM | 877 | C   | LEU | A | 115 | 3.619  | 53.896 | 60.870 | 1.00 | 22.95 |
| ATOM | 878 | O   | LEU | A | 115 | 3.042  | 54.162 | 61.924 | 1.00 | 22.70 |
| ATOM | 879 | CB  | LEU | A | 115 | 2.418  | 53.298 | 58.851 | 1.00 | 18.69 |
| ATOM | 880 | CG  | LEU | A | 115 | 1.844  | 52.219 | 57.960 | 1.00 | 24.36 |
| ATOM | 881 | CD1 | LEU | A | 115 | 0.784  | 52.871 | 57.078 | 1.00 | 26.30 |
| ATOM | 882 | CD2 | LEU | A | 115 | 2.954  | 51.654 | 57.070 | 1.00 | 21.90 |
| ATOM | 883 | N   | GLN | A | 116 | 4.573  | 54.621 | 60.358 | 1.00 | 19.91 |
| ATOM | 884 | CA  | GLN | A | 116 | 4.959  | 55.857 | 60.974 | 1.00 | 19.64 |
| ATOM | 885 | C   | GLN | A | 116 | 5.071  | 56.896 | 59.851 | 1.00 | 22.36 |
| ATOM | 886 | O   | GLN | A | 116 | 5.898  | 56.769 | 58.943 | 1.00 | 21.29 |
| ATOM | 887 | CB  | GLN | A | 116 | 6.195  | 55.857 | 61.891 | 1.00 | 21.78 |
| ATOM | 888 | CG  | GLN | A | 116 | 6.297  | 57.220 | 62.637 | 1.00 | 28.22 |
| ATOM | 889 | CD  | GLN | A | 116 | 7.539  | 57.423 | 63.481 | 1.00 | 33.89 |
| ATOM | 890 | OE1 | GLN | A | 116 | 8.458  | 56.585 | 63.489 | 1.00 | 21.37 |
| ATOM | 891 | NE2 | GLN | A | 116 | 7.569  | 58.557 | 64.198 | 1.00 | 25.06 |
| ATOM | 892 | N   | TRP | A | 117 | 4.207  | 57.898 | 59.926 | 1.00 | 21.50 |
| ATOM | 893 | CA  | TRP | A | 117 | 4.163  | 58.982 | 58.973 | 1.00 | 22.21 |
| ATOM | 894 | C   | TRP | A | 117 | 4.909  | 60.164 | 59.588 | 1.00 | 24.80 |
| ATOM | 895 | O   | TRP | A | 117 | 4.500  | 60.677 | 60.633 | 1.00 | 24.36 |
| ATOM | 896 | CB  | TRP | A | 117 | 2.706  | 59.380 | 58.730 | 1.00 | 20.63 |
| ATOM | 897 | CG  | TRP | A | 117 | 1.887  | 58.374 | 57.979 | 1.00 | 21.43 |
| ATOM | 898 | CD1 | TRP | A | 117 | 1.079  | 57.439 | 58.532 | 1.00 | 24.14 |
| ATOM | 899 | CD2 | TRP | A | 117 | 1.736  | 58.258 | 56.562 | 1.00 | 20.88 |
| ATOM | 900 | NE1 | TRP | A | 117 | 0.467  | 56.706 | 57.553 | 1.00 | 22.57 |
| ATOM | 901 | CE2 | TRP | A | 117 | 0.832  | 57.196 | 56.331 | 1.00 | 24.10 |
| ATOM | 902 | CE3 | TRP | A | 117 | 2.279  | 58.953 | 55.467 | 1.00 | 23.47 |
| ATOM | 903 | CZ2 | TRP | A | 117 | 0.450  | 56.806 | 55.038 | 1.00 | 24.69 |
| ATOM | 904 | CZ3 | TRP | A | 117 | 1.929  | 58.563 | 54.182 | 1.00 | 26.53 |
| ATOM | 905 | CH2 | TRP | A | 117 | 1.022  | 57.503 | 53.974 | 1.00 | 27.59 |
| ATOM | 906 | N   | LEU | A | 118 | 6.000  | 60.565 | 58.932 | 1.00 | 19.11 |
| ATOM | 907 | CA  | LEU | A | 118 | 6.864  | 61.652 | 59.372 | 1.00 | 20.20 |
| ATOM | 908 | C   | LEU | A | 118 | 6.594  | 62.936 | 58.603 | 1.00 | 29.18 |
| ATOM | 909 | O   | LEU | A | 118 | 6.422  | 62.907 | 57.379 | 1.00 | 29.44 |
| ATOM | 910 | CB  | LEU | A | 118 | 8.364  | 61.287 | 59.137 | 1.00 | 21.47 |
| ATOM | 911 | CG  | LEU | A | 118 | 8.985  | 60.284 | 60.141 | 1.00 | 28.52 |
| ATOM | 912 | CD1 | LEU | A | 118 | 8.137  | 59.016 | 60.275 | 1.00 | 30.03 |
| ATOM | 913 | CD2 | LEU | A | 118 | 10.410 | 59.939 | 59.716 | 1.00 | 27.52 |
| ATOM | 914 | N   | THR | A | 119 | 6.573  | 64.076 | 59.305 | 1.00 | 23.98 |
| ATOM | 915 | CA  | THR | A | 119 | 6.379  | 65.362 | 58.636 | 1.00 | 19.34 |
| ATOM | 916 | C   | THR | A | 119 | 7.776  | 65.731 | 58.183 | 1.00 | 23.45 |
| ATOM | 917 | O   | THR | A | 119 | 8.736  | 65.253 | 58.783 | 1.00 | 24.77 |
| ATOM | 918 | CB  | THR | A | 119 | 5.910  | 66.402 | 59.682 | 1.00 | 26.76 |
| ATOM | 919 | OG1 | THR | A | 119 | 6.915  | 66.529 | 60.673 | 1.00 | 27.33 |
| ATOM | 920 | CG2 | THR | A | 119 | 4.637  | 65.950 | 60.390 | 1.00 | 28.42 |
| ATOM | 921 | N   | PRO | A | 120 | 7.933  | 66.565 | 57.151 | 1.00 | 22.29 |
| ATOM | 922 | CA  | PRO | A | 120 | 9.255  | 66.927 | 56.678 | 1.00 | 22.30 |



|      |     |     |     |   |     |        |        |        |      |        |
|------|-----|-----|-----|---|-----|--------|--------|--------|------|--------|
| ATOM | 923 | C   | PRO | A | 120 | 10.178 | 67.419 | 57.800 | 1.00 | 28.55  |
| ATOM | 924 | O   | PRO | A | 120 | 11.404 | 67.260 | 57.754 | 1.00 | 27.54  |
| ATOM | 925 | CB  | PRO | A | 120 | 9.059  | 68.024 | 55.624 | 1.00 | 23.05  |
| ATOM | 926 | CG  | PRO | A | 120 | 7.581  | 68.150 | 55.384 | 1.00 | 24.12  |
| ATOM | 927 | CD  | PRO | A | 120 | 6.876  | 67.282 | 56.407 | 1.00 | 21.87  |
| ATOM | 928 | N   | GLU | A | 121 | 9.583  | 68.022 | 58.822 | 1.00 | 28.60  |
| ATOM | 929 | CA  | GLU | A | 121 | 10.366 | 68.529 | 59.937 | 1.00 | 31.89  |
| ATOM | 930 | C   | GLU | A | 121 | 11.104 | 67.394 | 60.658 | 1.00 | 37.79  |
| ATOM | 931 | O   | GLU | A | 121 | 12.205 | 67.554 | 61.198 | 1.00 | 35.72  |
| ATOM | 932 | CB  | GLU | A | 121 | 9.442  | 69.247 | 60.938 | 1.00 | 34.44  |
| ATOM | 933 | CG  | GLU | A | 121 | 8.757  | 70.526 | 60.397 | 1.00 | 61.71  |
| ATOM | 934 | CD  | GLU | A | 121 | 7.773  | 70.370 | 59.250 | 1.00 | 95.37  |
| ATOM | 935 | OE1 | GLU | A | 121 | 6.808  | 69.624 | 59.252 | 1.00 | 50.70  |
| ATOM | 936 | OE2 | GLU | A | 121 | 8.033  | 71.193 | 58.262 | 1.00 | 100.00 |
| ATOM | 937 | N   | GLN | A | 122 | 10.456 | 66.228 | 60.673 | 1.00 | 33.10  |
| ATOM | 938 | CA  | GLN | A | 122 | 11.011 | 65.066 | 61.339 | 1.00 | 30.63  |
| ATOM | 939 | C   | GLN | A | 122 | 12.104 | 64.392 | 60.538 | 1.00 | 33.25  |
| ATOM | 940 | O   | GLN | A | 122 | 12.637 | 63.388 | 60.962 | 1.00 | 33.00  |
| ATOM | 941 | CB  | GLN | A | 122 | 9.905  | 64.039 | 61.637 | 1.00 | 30.70  |
| ATOM | 942 | CG  | GLN | A | 122 | 8.966  | 64.462 | 62.774 | 1.00 | 23.20  |
| ATOM | 943 | CD  | GLN | A | 122 | 7.703  | 63.620 | 62.818 | 1.00 | 27.73  |
| ATOM | 944 | OE1 | GLN | A | 122 | 6.781  | 63.798 | 62.016 | 1.00 | 34.90  |
| ATOM | 945 | NE2 | GLN | A | 122 | 7.655  | 62.689 | 63.757 | 1.00 | 30.55  |
| ATOM | 946 | N   | THR | A | 123 | 12.427 | 64.912 | 59.356 | 1.00 | 29.61  |
| ATOM | 947 | CA  | THR | A | 123 | 13.438 | 64.288 | 58.495 | 1.00 | 27.96  |
| ATOM | 948 | C   | THR | A | 123 | 14.730 | 65.030 | 58.506 | 1.00 | 31.63  |
| ATOM | 949 | O   | THR | A | 123 | 14.831 | 66.111 | 59.060 | 1.00 | 34.46  |
| ATOM | 950 | CB  | THR | A | 123 | 12.966 | 64.183 | 57.029 | 1.00 | 24.54  |
| ATOM | 951 | OG1 | THR | A | 123 | 12.855 | 65.504 | 56.515 | 1.00 | 28.43  |
| ATOM | 952 | CG2 | THR | A | 123 | 11.594 | 63.521 | 56.985 | 1.00 | 18.48  |
| ATOM | 953 | N   | SER | A | 124 | 15.712 | 64.440 | 57.870 | 1.00 | 24.71  |
| ATOM | 954 | CA  | SER | A | 124 | 16.980 | 65.088 | 57.814 | 1.00 | 25.71  |
| ATOM | 955 | C   | SER | A | 124 | 16.886 | 66.308 | 56.900 | 1.00 | 34.45  |
| ATOM | 956 | O   | SER | A | 124 | 17.399 | 67.377 | 57.227 | 1.00 | 34.98  |
| ATOM | 957 | CB  | SER | A | 124 | 18.094 | 64.182 | 57.317 | 1.00 | 25.78  |
| ATOM | 958 | OG  | SER | A | 124 | 18.268 | 63.099 | 58.177 | 1.00 | 34.37  |
| ATOM | 959 | N   | GLY | A | 125 | 16.221 | 66.110 | 55.756 | 1.00 | 32.47  |
| ATOM | 960 | CA  | GLY | A | 125 | 16.042 | 67.119 | 54.717 | 1.00 | 33.54  |
| ATOM | 961 | C   | GLY | A | 125 | 15.086 | 68.279 | 55.024 | 1.00 | 38.01  |
| ATOM | 962 | O   | GLY | A | 125 | 15.226 | 69.371 | 54.450 | 1.00 | 35.01  |
| ATOM | 963 | N   | LYS | A | 126 | 14.100 | 68.055 | 55.893 | 1.00 | 32.87  |
| ATOM | 964 | CA  | LYS | A | 126 | 13.181 | 69.126 | 56.236 | 1.00 | 30.74  |
| ATOM | 965 | C   | LYS | A | 126 | 12.281 | 69.626 | 55.101 | 1.00 | 34.13  |
| ATOM |     |     |     |   |     |        |        |        |      |        |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 981  | N   | HIS | A | 128 | 10.729 | 67.260 | 52.730 | 1.00 | 32.31 |
| ATOM | 982  | CA  | HIS | A | 128 | 9.786  | 66.221 | 52.395 | 1.00 | 29.92 |
| ATOM | 983  | C   | HIS | A | 128 | 9.400  | 65.337 | 53.570 | 1.00 | 27.82 |
| ATOM | 984  | O   | HIS | A | 128 | 10.117 | 65.179 | 54.549 | 1.00 | 29.92 |
| ATOM | 985  | CB  | HIS | A | 128 | 10.345 | 65.324 | 51.308 | 1.00 | 29.24 |
| ATOM | 986  | CG  | HIS | A | 128 | 10.843 | 66.080 | 50.152 | 1.00 | 31.61 |
| ATOM | 987  | ND1 | HIS | A | 128 | 9.978  | 66.601 | 49.205 | 1.00 | 33.89 |
| ATOM | 988  | CD2 | HIS | A | 128 | 12.113 | 66.358 | 49.795 | 1.00 | 34.18 |
| ATOM | 989  | CE1 | HIS | A | 128 | 10.738 | 67.176 | 48.294 | 1.00 | 33.86 |
| ATOM | 990  | NE2 | HIS | A | 128 | 12.030 | 67.053 | 48.618 | 1.00 | 34.37 |
| ATOM | 991  | N   | PRO | A | 129 | 8.261  | 64.747 | 53.430 | 1.00 | 21.92 |
| ATOM | 992  | CA  | PRO | A | 129 | 7.756  | 63.846 | 54.424 | 1.00 | 21.51 |
| ATOM | 993  | C   | PRO | A | 129 | 8.419  | 62.474 | 54.216 | 1.00 | 26.61 |
| ATOM | 994  | O   | PRO | A | 129 | 9.302  | 62.284 | 53.376 | 1.00 | 25.02 |
| ATOM | 995  | CB  | PRO | A | 129 | 6.265  | 63.736 | 54.162 | 1.00 | 21.80 |
| ATOM | 996  | CG  | PRO | A | 129 | 6.098  | 64.059 | 52.690 | 1.00 | 28.71 |
| ATOM | 997  | CD  | PRO | A | 129 | 7.353  | 64.818 | 52.263 | 1.00 | 23.90 |
| ATOM | 998  | N   | TYR | A | 130 | 8.016  | 61.498 | 54.998 | 1.00 | 22.26 |
| ATOM | 999  | CA  | TYR | A | 130 | 8.646  | 60.195 | 54.881 | 1.00 | 20.30 |
| ATOM | 1000 | C   | TYR | A | 130 | 7.747  | 59.148 | 55.492 | 1.00 | 23.74 |
| ATOM | 1001 | O   | TYR | A | 130 | 7.022  | 59.381 | 56.442 | 1.00 | 23.54 |
| ATOM | 1002 | CB  | TYR | A | 130 | 9.959  | 60.250 | 55.663 | 1.00 | 20.15 |
| ATOM | 1003 | CG  | TYR | A | 130 | 10.909 | 59.072 | 55.574 | 1.00 | 23.26 |
| ATOM | 1004 | CD1 | TYR | A | 130 | 10.623 | 57.805 | 56.104 | 1.00 | 23.27 |
| ATOM | 1005 | CD2 | TYR | A | 130 | 12.148 | 59.271 | 54.966 | 1.00 | 24.16 |
| ATOM | 1006 | CE1 | TYR | A | 130 | 11.555 | 56.765 | 56.013 | 1.00 | 20.09 |
| ATOM | 1007 | CE2 | TYR | A | 130 | 13.100 | 58.255 | 54.888 | 1.00 | 23.94 |
| ATOM | 1008 | CZ  | TYR | A | 130 | 12.795 | 57.001 | 55.410 | 1.00 | 19.50 |
| ATOM | 1009 | OH  | TYR | A | 130 | 13.751 | 56.053 | 55.281 | 1.00 | 24.55 |
| ATOM | 1010 | N   | LEU | A | 131 | 7.764  | 57.970 | 54.948 | 1.00 | 21.39 |
| ATOM | 1011 | CA  | LEU | A | 131 | 6.916  | 56.975 | 55.551 | 1.00 | 23.29 |
| ATOM | 1012 | C   | LEU | A | 131 | 7.671  | 55.654 | 55.583 | 1.00 | 26.48 |
| ATOM | 1013 | O   | LEU | A | 131 | 8.450  | 55.368 | 54.658 | 1.00 | 22.90 |
| ATOM | 1014 | CB  | LEU | A | 131 | 5.632  | 56.805 | 54.721 | 1.00 | 22.31 |
| ATOM | 1015 | CG  | LEU | A | 131 | 4.960  | 55.462 | 54.943 | 1.00 | 24.82 |
| ATOM | 1016 | CD1 | LEU | A | 131 | 4.060  | 55.574 | 56.168 | 1.00 | 24.09 |
| ATOM | 1017 | CD2 | LEU | A | 131 | 4.166  | 55.056 | 53.690 | 1.00 | 23.63 |
| ATOM | 1018 | N   | PHE | A | 132 | 7.463  | 54.866 | 56.631 | 1.00 | 24.01 |
| ATOM | 1019 | CA  | PHE | A | 132 | 8.101  | 53.539 | 56.711 | 1.00 | 23.69 |
| ATOM | 1020 | C   | PHE | A | 132 | 7.231  | 52.575 | 57.474 | 1.00 | 23.59 |
| ATOM | 1021 | O   | PHE | A | 132 | 6.529  | 52.952 | 58.394 | 1.00 | 20.95 |
| ATOM | 1022 | CB  | PHE | A | 132 | 9.545  | 53.507 | 57.253 | 1.00 | 25.79 |
| ATOM | 1023 | CG  | PHE | A | 132 | 9.654  | 53.806 | 58.740 | 1.00 | 26.81 |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 1039 | CB  | GLN | A | 134 | 7.966  | 48.415 | 61.526 | 1.00 | 16.26 |
| ATOM | 1040 | CG  | GLN | A | 134 | 8.392  | 47.346 | 62.549 | 1.00 | 24.87 |
| ATOM | 1041 | CD  | GLN | A | 134 | 9.424  | 46.414 | 61.955 | 1.00 | 36.09 |
| ATOM | 1042 | OE1 | GLN | A | 134 | 10.363 | 46.862 | 61.280 | 1.00 | 25.12 |
| ATOM | 1043 | NE2 | GLN | A | 134 | 9.242  | 45.111 | 62.187 | 1.00 | 30.48 |
| ATOM | 1044 | N   | CYS | A | 135 | 6.076  | 45.647 | 60.013 | 1.00 | 15.84 |
| ATOM | 1045 | CA  | CYS | A | 135 | 5.025  | 44.712 | 60.313 | 1.00 | 16.52 |
| ATOM | 1046 | C   | CYS | A | 135 | 5.298  | 43.683 | 61.381 | 1.00 | 18.38 |
| ATOM | 1047 | O   | CYS | A | 135 | 4.354  | 43.170 | 61.995 | 1.00 | 19.10 |
| ATOM | 1048 | CB  | CYS | A | 135 | 4.649  | 43.908 | 59.067 | 1.00 | 20.50 |
| ATOM | 1049 | SG  | CYS | A | 135 | 4.051  | 44.971 | 57.762 | 1.00 | 25.25 |
| ATOM | 1050 | N   | GLN | A | 136 | 6.545  | 43.284 | 61.564 | 1.00 | 16.69 |
| ATOM | 1051 | CA  | GLN | A | 136 | 6.756  | 42.242 | 62.572 | 1.00 | 16.53 |
| ATOM | 1052 | C   | GLN | A | 136 | 6.454  | 42.824 | 63.926 | 1.00 | 20.04 |
| ATOM | 1053 | O   | GLN | A | 136 | 6.853  | 43.946 | 64.194 | 1.00 | 21.71 |
| ATOM | 1054 | CB  | GLN | A | 136 | 8.204  | 41.703 | 62.520 | 1.00 | 18.54 |
| ATOM | 1055 | CG  | GLN | A | 136 | 8.488  | 40.565 | 63.533 | 1.00 | 16.78 |
| ATOM | 1056 | CD  | GLN | A | 136 | 9.930  | 40.052 | 63.434 | 1.00 | 27.57 |
| ATOM | 1057 | OE1 | GLN | A | 136 | 10.835 | 40.746 | 62.930 | 1.00 | 19.61 |
| ATOM | 1058 | NE2 | GLN | A | 136 | 10.141 | 38.826 | 63.903 | 1.00 | 25.09 |
| ATOM | 1059 | N   | ALA | A | 137 | 5.730  | 42.087 | 64.769 | 1.00 | 16.79 |
| ATOM | 1060 | CA  | ALA | A | 137 | 5.243  | 40.724 | 64.514 | 1.00 | 16.58 |
| ATOM | 1061 | C   | ALA | A | 137 | 3.931  | 40.636 | 63.807 | 1.00 | 20.75 |
| ATOM | 1062 | O   | ALA | A | 137 | 3.798  | 39.912 | 62.836 | 1.00 | 19.63 |
| ATOM | 1063 | CB  | ALA | A | 137 | 5.087  | 39.918 | 65.813 | 1.00 | 16.76 |
| ATOM | 1064 | N   | ILE | A | 138 | 2.951  | 41.338 | 64.321 | 1.00 | 18.31 |
| ATOM | 1065 | CA  | ILE | A | 138 | 1.647  | 41.247 | 63.721 | 1.00 | 18.68 |
| ATOM | 1066 | C   | ILE | A | 138 | 1.065  | 42.566 | 63.294 | 1.00 | 19.68 |
| ATOM | 1067 | O   | ILE | A | 138 | -0.053 | 42.896 | 63.633 | 1.00 | 21.65 |
| ATOM | 1068 | CB  | ILE | A | 138 | 0.727  | 40.532 | 64.692 | 1.00 | 20.75 |
| ATOM | 1069 | CG1 | ILE | A | 138 | 0.761  | 41.275 | 66.024 | 1.00 | 21.55 |
| ATOM | 1070 | CG2 | ILE | A | 138 | 1.241  | 39.124 | 64.882 | 1.00 | 17.75 |
| ATOM | 1071 | CD1 | ILE | A | 138 | -0.211 | 40.698 | 67.044 | 1.00 | 23.44 |
| ATOM | 1072 | N   | HIS | A | 139 | 1.789  | 43.309 | 62.525 | 1.00 | 19.15 |
| ATOM | 1073 | CA  | HIS | A | 139 | 1.231  | 44.581 | 62.113 | 1.00 | 19.05 |
| ATOM | 1074 | C   | HIS | A | 139 | 0.899  | 44.615 | 60.644 | 1.00 | 23.60 |
| ATOM | 1075 | O   | HIS | A | 139 | 0.427  | 45.604 | 60.127 | 1.00 | 25.90 |
| ATOM | 1076 | CB  | HIS | A | 139 | 2.149  | 45.781 | 62.471 | 1.00 | 19.09 |
| ATOM | 1077 | CG  | HIS | A | 139 | 2.429  | 45.870 | 63.961 | 1.00 | 21.83 |
| ATOM | 1078 | ND1 | HIS | A | 139 | 1.476  | 46.324 | 64.872 | 1.00 | 22.32 |
| ATOM | 1079 | CD2 | HIS | A | 139 | 3.547  | 45.567 | 64.661 | 1.00 | 21.82 |
| ATOM | 1080 | CE1 | HIS | A | 139 | 2.022  | 46.253 | 66.072 | 1.00 | 21.72 |
| ATOM | 1081 | NE2 | HIS | A | 139 | 3.259  | 45.811 | 65.980 | 1.00 | 21.41 |
| ATOM | 1082 | N   | CYS | A | 140 | 1.175  | 43.545 | 59.942 | 1.00 | 21.39 |
| ATOM | 1083 | CA  | CYS | A | 140 | 0.854  | 43.573 | 58.525 | 1.00 | 21.71 |
| ATOM | 1084 | C   | CYS | A | 140 | -0.630 | 43.848 | 58.327 | 1.00 | 20.64 |
| ATOM | 1085 | O   | CYS | A | 140 | -1.071 | 44.542 | 57.405 | 1.00 | 21.98 |
| ATOM | 1086 | CB  | CYS | A | 140 | 1.237  | 42.260 | 57.823 | 1.00 | 22.30 |
| ATOM | 1087 | SG  | CYS | A | 140 | 1.089  | 42.457 | 56.029 | 1.00 | 27.57 |
| ATOM | 1088 | N   | ARG | A | 141 | -1.384 | 43.259 | 59.232 | 1.00 | 18.28 |
| ATOM | 1089 | CA  | ARG | A | 141 | -2.819 | 43.369 | 59.261 | 1.00 | 20.32 |
| ATOM | 1090 | C   | ARG | A | 141 | -3.265 | 44.823 | 59.352 | 1.00 | 27.93 |
| ATOM | 1091 | O   | ARG | A | 141 | -4.438 | 45.135 | 59.078 | 1.00 | 29.72 |
| ATOM | 1092 | CB  | ARG | A | 141 | -3.436 | 42.518 | 60.369 | 1.00 | 16.68 |
| ATOM | 1093 | CG  | ARG | A | 141 | -3.035 | 42.944 | 61.781 | 1.00 | 18.27 |
| ATOM | 1094 | CD  | ARG | A | 141 | -3.571 | 41.985 | 62.866 | 1.00 | 15.44 |
| ATOM | 1095 | NE  | ARG | A | 141 | -2.857 | 40.717 | 62.896 | 1.00 | 20.15 |
| ATOM | 1096 | CZ  | ARG | A | 141 | -2.996 | 39.785 | 63.813 | 1.00 | 20.72 |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 1097 | NH1 | ARG | A | 141 | -3.825 | 39.908 | 64.827 | 1.00 | 16.67 |
| ATOM | 1098 | NH2 | ARG | A | 141 | -2.258 | 38.692 | 63.685 | 1.00 | 22.83 |
| ATOM | 1099 | N   | ALA | A | 142 | -2.314 | 45.707 | 59.754 | 1.00 | 18.15 |
| ATOM | 1100 | CA  | ALA | A | 142 | -2.599 | 47.127 | 59.901 | 1.00 | 17.64 |
| ATOM | 1101 | C   | ALA | A | 142 | -2.265 | 47.823 | 58.619 | 1.00 | 22.89 |
| ATOM | 1102 | O   | ALA | A | 142 | -2.296 | 49.024 | 58.506 | 1.00 | 22.38 |
| ATOM | 1103 | CB  | ALA | A | 142 | -1.908 | 47.771 | 61.085 | 1.00 | 17.04 |
| ATOM | 1104 | N   | ILE | A | 143 | -1.925 | 47.041 | 57.621 | 1.00 | 24.40 |
| ATOM | 1105 | CA  | ILE | A | 143 | -1.634 | 47.632 | 56.341 | 1.00 | 25.97 |
| ATOM | 1106 | C   | ILE | A | 143 | -2.641 | 47.117 | 55.334 | 1.00 | 33.49 |
| ATOM | 1107 | O   | ILE | A | 143 | -3.259 | 47.865 | 54.585 | 1.00 | 36.37 |
| ATOM | 1108 | CB  | ILE | A | 143 | -0.222 | 47.447 | 55.839 | 1.00 | 29.94 |
| ATOM | 1109 | CG1 | ILE | A | 143 | 0.791  | 47.972 | 56.853 | 1.00 | 29.88 |
| ATOM | 1110 | CG2 | ILE | A | 143 | -0.094 | 48.232 | 54.533 | 1.00 | 33.06 |
| ATOM | 1111 | CD1 | ILE | A | 143 | 2.224  | 47.722 | 56.389 | 1.00 | 26.42 |
| ATOM | 1112 | N   | LEU | A | 144 | -2.843 | 45.822 | 55.350 | 1.00 | 28.38 |
| ATOM | 1113 | CA  | LEU | A | 144 | -3.815 | 45.204 | 54.438 | 1.00 | 29.40 |
| ATOM | 1114 | C   | LEU | A | 144 | -4.421 | 43.917 | 55.030 | 1.00 | 33.99 |
| ATOM | 1115 | O   | LEU | A | 144 | -3.928 | 43.349 | 56.037 | 1.00 | 30.51 |
| ATOM | 1116 | CB  | LEU | A | 144 | -3.213 | 44.969 | 53.037 | 1.00 | 30.43 |
| ATOM | 1117 | CG  | LEU | A | 144 | -1.868 | 44.266 | 53.111 | 1.00 | 33.80 |
| ATOM | 1118 | CD1 | LEU | A | 144 | -2.073 | 42.761 | 53.007 | 1.00 | 35.20 |
| ATOM | 1119 | CD2 | LEU | A | 144 | -0.935 | 44.758 | 52.023 | 1.00 | 38.26 |
| ATOM | 1120 | N   | PRO | A | 145 | -5.507 | 43.446 | 54.432 | 1.00 | 27.43 |
| ATOM | 1121 | CA  | PRO | A | 145 | -6.094 | 42.259 | 54.979 | 1.00 | 25.19 |
| ATOM | 1122 | C   | PRO | A | 145 | -5.294 | 41.059 | 54.513 | 1.00 | 23.80 |
| ATOM | 1123 | O   | PRO | A | 145 | -4.832 | 41.009 | 53.376 | 1.00 | 23.96 |
| ATOM | 1124 | CB  | PRO | A | 145 | -7.567 | 42.266 | 54.566 | 1.00 | 27.07 |
| ATOM | 1125 | CG  | PRO | A | 145 | -7.810 | 43.609 | 53.886 | 1.00 | 31.08 |
| ATOM | 1126 | CD  | PRO | A | 145 | -6.445 | 44.131 | 53.505 | 1.00 | 26.31 |
| ATOM | 1127 | N   | CYS | A | 146 | -5.080 | 40.145 | 55.448 | 1.00 | 23.01 |
| ATOM | 1128 | CA  | CYS | A | 146 | -4.272 | 38.956 | 55.215 | 1.00 | 24.70 |
| ATOM | 1129 | C   | CYS | A | 146 | -4.329 | 37.973 | 56.367 | 1.00 | 28.20 |
| ATOM | 1130 | O   | CYS | A | 146 | -4.966 | 38.211 | 57.413 | 1.00 | 23.14 |
| ATOM | 1131 | CB  | CYS | A | 146 | -2.793 | 39.335 | 55.036 | 1.00 | 25.42 |
| ATOM | 1132 | SG  | CYS | A | 146 | -2.164 | 40.274 | 56.463 | 1.00 | 31.88 |
| ATOM | 1133 | N   | GLN | A | 147 | -3.647 | 36.843 | 56.134 | 1.00 | 22.82 |
| ATOM | 1134 | CA  | GLN | A | 147 | -3.522 | 35.796 | 57.127 | 1.00 | 23.08 |
| ATOM | 1135 | C   | GLN | A | 147 | -2.238 | 36.197 | 57.832 | 1.00 | 28.00 |
| ATOM | 1136 | O   | GLN | A | 147 | -1.131 | 35.841 | 57.415 | 1.00 | 25.08 |
| ATOM | 1137 | CB  | GLN | A | 147 | -3.346 | 34.427 | 56.449 | 1.00 | 24.85 |
| ATOM | 1138 | CG  | GLN | A | 147 | -4.671 | 33.762 | 56.084 | 1.00 | 19.17 |
| ATOM | 1139 | CD  | GLN | A | 147 | -4.391 | 32.428 | 55.427 | 1.00 | 25.96 |
| ATOM |      |     |     |   |     |        |        |        |      |       |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 1155 | OG1 | THR | A | 149 | 0.577  | 32.168 | 61.421 | 1.00 | 24.67 |
| ATOM | 1156 | CG2 | THR | A | 149 | -0.979 | 32.910 | 59.680 | 1.00 | 23.64 |
| ATOM | 1157 | N   | PRO | A | 150 | 2.921  | 33.765 | 60.686 | 1.00 | 21.90 |
| ATOM | 1158 | CA  | PRO | A | 150 | 4.159  | 33.323 | 60.016 | 1.00 | 19.21 |
| ATOM | 1159 | C   | PRO | A | 150 | 4.018  | 31.886 | 59.479 | 1.00 | 21.32 |
| ATOM | 1160 | O   | PRO | A | 150 | 4.898  | 31.352 | 58.829 | 1.00 | 18.90 |
| ATOM | 1161 | CB  | PRO | A | 150 | 5.260  | 33.356 | 61.103 | 1.00 | 19.24 |
| ATOM | 1162 | CG  | PRO | A | 150 | 4.544  | 33.455 | 62.444 | 1.00 | 20.32 |
| ATOM | 1163 | CD  | PRO | A | 150 | 3.125  | 33.922 | 62.168 | 1.00 | 20.18 |
| ATOM | 1164 | N   | SER | A | 151 | 2.902  | 31.226 | 59.771 | 1.00 | 18.68 |
| ATOM | 1165 | CA  | SER | A | 151 | 2.737  | 29.862 | 59.276 | 1.00 | 20.66 |
| ATOM | 1166 | C   | SER | A | 151 | 2.351  | 29.863 | 57.820 | 1.00 | 22.40 |
| ATOM | 1167 | O   | SER | A | 151 | 2.295  | 28.836 | 57.199 | 1.00 | 26.24 |
| ATOM | 1168 | CB  | SER | A | 151 | 1.674  | 29.117 | 60.057 | 1.00 | 25.01 |
| ATOM | 1169 | OG  | SER | A | 151 | 0.444  | 29.814 | 59.897 | 1.00 | 32.09 |
| ATOM | 1170 | N   | VAL | A | 152 | 2.086  | 31.017 | 57.282 | 1.00 | 18.17 |
| ATOM | 1171 | CA  | VAL | A | 152 | 1.696  | 31.105 | 55.899 | 1.00 | 20.54 |
| ATOM | 1172 | C   | VAL | A | 152 | 2.740  | 31.874 | 55.088 | 1.00 | 26.40 |
| ATOM | 1173 | O   | VAL | A | 152 | 3.159  | 32.955 | 55.494 | 1.00 | 25.43 |
| ATOM | 1174 | CB  | VAL | A | 152 | 0.307  | 31.756 | 55.773 | 1.00 | 22.01 |
| ATOM | 1175 | CG1 | VAL | A | 152 | 0.000  | 32.092 | 54.316 | 1.00 | 21.07 |
| ATOM | 1176 | CG2 | VAL | A | 152 | -0.742 | 30.818 | 56.325 | 1.00 | 21.78 |
| ATOM | 1177 | N   | LYS | A | 153 | 3.163  | 31.316 | 53.934 | 1.00 | 21.69 |
| ATOM | 1178 | CA  | LYS | A | 153 | 4.146  | 31.985 | 53.101 | 1.00 | 20.64 |
| ATOM | 1179 | C   | LYS | A | 153 | 3.606  | 32.223 | 51.720 | 1.00 | 25.15 |
| ATOM | 1180 | O   | LYS | A | 153 | 3.041  | 31.329 | 51.114 | 1.00 | 27.06 |
| ATOM | 1181 | CB  | LYS | A | 153 | 5.455  | 31.218 | 53.016 | 1.00 | 24.18 |
| ATOM | 1182 | CG  | LYS | A | 153 | 6.159  | 31.061 | 54.360 | 1.00 | 29.97 |
| ATOM | 1183 | CD  | LYS | A | 153 | 7.582  | 30.546 | 54.220 | 1.00 | 19.10 |
| ATOM | 1184 | CE  | LYS | A | 153 | 8.276  | 30.287 | 55.546 | 1.00 | 24.45 |
| ATOM | 1185 | NZ  | LYS | A | 153 | 9.760  | 30.289 | 55.457 | 1.00 | 21.92 |
| ATOM | 1186 | N   | LEU | A | 154 | 3.768  | 33.438 | 51.213 | 1.00 | 22.90 |
| ATOM | 1187 | CA  | LEU | A | 154 | 3.286  | 33.772 | 49.876 | 1.00 | 22.75 |
| ATOM | 1188 | C   | LEU | A | 154 | 4.280  | 34.594 | 49.091 | 1.00 | 23.26 |
| ATOM | 1189 | O   | LEU | A | 154 | 5.225  | 35.207 | 49.624 | 1.00 | 21.95 |
| ATOM | 1190 | CB  | LEU | A | 154 | 1.989  | 34.615 | 49.972 | 1.00 | 23.48 |
| ATOM | 1191 | CG  | LEU | A | 154 | 2.246  | 35.948 | 50.729 | 1.00 | 29.06 |
| ATOM | 1192 | CD1 | LEU | A | 154 | 1.385  | 37.086 | 50.200 | 1.00 | 29.05 |
| ATOM | 1193 | CD2 | LEU | A | 154 | 1.986  | 35.788 | 52.225 | 1.00 | 26.55 |
| ATOM | 1194 | N   | THR | A | 155 | 4.033  | 34.653 | 47.791 | 1.00 | 22.63 |
| ATOM | 1195 | CA  | THR | A | 155 | 4.862  | 35.499 | 46.940 | 1.00 | 25.54 |
| ATOM | 1196 | C   | THR | A | 155 | 4.088  | 36.820 | 46.772 | 1.00 | 26.35 |
| ATOM | 1197 | O   | THR | A | 155 | 2.929  | 36.943 | 47.190 | 1.00 | 25.33 |
| ATOM | 1198 | CB  | THR | A | 155 | 5.122  | 34.931 | 45.526 | 1.00 | 26.50 |
| ATOM | 1199 | OG1 | THR | A | 155 | 3.937  | 34.294 | 45.141 | 1.00 | 31.87 |
| ATOM | 1200 | CG2 | THR | A | 155 | 6.327  | 33.991 | 45.488 | 1.00 | 21.48 |
| ATOM | 1201 | N   | TYR | A | 156 | 4.721  | 37.802 | 46.154 | 1.00 | 23.09 |
| ATOM | 1202 | CA  | TYR | A | 156 | 4.021  | 39.040 | 45.943 | 1.00 | 22.25 |
| ATOM | 1203 | C   | TYR | A | 156 | 4.631  | 39.924 | 44.889 | 1.00 | 24.76 |
| ATOM | 1204 | O   | TYR | A | 156 | 5.846  | 39.919 | 44.601 | 1.00 | 28.65 |
| ATOM | 1205 | CB  | TYR | A | 156 | 3.735  | 39.831 | 47.252 | 1.00 | 22.99 |
| ATOM | 1206 | CG  | TYR | A | 156 | 4.853  | 40.754 | 47.751 | 1.00 | 24.46 |
| ATOM | 1207 | CD1 | TYR | A | 156 | 4.992  | 42.048 | 47.246 | 1.00 | 26.47 |
| ATOM | 1208 | CD2 | TYR | A | 156 | 5.744  | 40.356 | 48.755 | 1.00 | 22.08 |
| ATOM | 1209 | CE1 | TYR | A | 156 | 6.003  | 42.894 | 47.704 | 1.00 | 27.20 |
| ATOM | 1210 | CE2 | TYR | A | 156 | 6.755  | 41.194 | 49.242 | 1.00 | 19.36 |
| ATOM | 1211 | CZ  | TYR | A | 156 | 6.874  | 42.476 | 48.709 | 1.00 | 28.26 |
| ATOM | 1212 | OH  | TYR | A | 156 | 7.819  | 43.341 | 49.176 | 1.00 | 23.92 |



|      |      |     |     |   |     |        |        |        |      |        |
|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
| ATOM | 1213 | N   | THR | A | 157 | 3.737  | 40.711 | 44.325 | 1.00 | 20.53  |
| ATOM | 1214 | CA  | THR | A | 157 | 4.079  | 41.726 | 43.358 | 1.00 | 22.66  |
| ATOM | 1215 | C   | THR | A | 157 | 3.374  | 42.996 | 43.844 | 1.00 | 27.95  |
| ATOM | 1216 | O   | THR | A | 157 | 2.300  | 42.941 | 44.469 | 1.00 | 27.60  |
| ATOM | 1217 | CB  | THR | A | 157 | 3.660  | 41.345 | 41.931 | 1.00 | 36.12  |
| ATOM | 1218 | OG1 | THR | A | 157 | 2.311  | 40.913 | 41.927 | 1.00 | 35.88  |
| ATOM | 1219 | CG2 | THR | A | 157 | 4.528  | 40.177 | 41.502 | 1.00 | 31.47  |
| ATOM | 1220 | N   | ALA | A | 158 | 3.984  | 44.136 | 43.604 | 1.00 | 26.56  |
| ATOM | 1221 | CA  | ALA | A | 158 | 3.357  | 45.363 | 44.034 | 1.00 | 28.25  |
| ATOM | 1222 | C   | ALA | A | 158 | 3.661  | 46.555 | 43.115 | 1.00 | 33.79  |
| ATOM | 1223 | O   | ALA | A | 158 | 4.737  | 46.682 | 42.469 | 1.00 | 31.04  |
| ATOM | 1224 | CB  | ALA | A | 158 | 3.749  | 45.700 | 45.460 | 1.00 | 26.89  |
| ATOM | 1225 | N   | GLU | A | 159 | 2.693  | 47.453 | 43.081 | 1.00 | 30.94  |
| ATOM | 1226 | CA  | GLU | A | 159 | 2.863  | 48.658 | 42.328 | 1.00 | 32.37  |
| ATOM | 1227 | C   | GLU | A | 159 | 2.434  | 49.789 | 43.226 | 1.00 | 31.24  |
| ATOM | 1228 | O   | GLU | A | 159 | 1.311  | 49.803 | 43.735 | 1.00 | 29.85  |
| ATOM | 1229 | CB  | GLU | A | 159 | 2.118  | 48.680 | 40.993 | 1.00 | 35.41  |
| ATOM | 1230 | CG  | GLU | A | 159 | 1.749  | 47.300 | 40.444 | 1.00 | 59.87  |
| ATOM | 1231 | CD  | GLU | A | 159 | 0.983  | 47.438 | 39.160 | 1.00 | 98.76  |
| ATOM | 1232 | OE1 | GLU | A | 159 | -0.110 | 47.979 | 39.091 | 1.00 | 78.51  |
| ATOM | 1233 | OE2 | GLU | A | 159 | 1.636  | 46.958 | 38.126 | 1.00 | 100.00 |
| ATOM | 1234 | N   | VAL | A | 160 | 3.337  | 50.714 | 43.472 | 1.00 | 28.73  |
| ATOM | 1235 | CA  | VAL | A | 160 | 2.915  | 51.778 | 44.352 | 1.00 | 29.43  |
| ATOM | 1236 | C   | VAL | A | 160 | 3.180  | 53.148 | 43.786 | 1.00 | 29.09  |
| ATOM | 1237 | O   | VAL | A | 160 | 4.292  | 53.442 | 43.354 | 1.00 | 27.09  |
| ATOM | 1238 | CB  | VAL | A | 160 | 3.370  | 51.589 | 45.785 | 1.00 | 33.76  |
| ATOM | 1239 | CG1 | VAL | A | 160 | 4.212  | 50.321 | 45.892 | 1.00 | 33.85  |
| ATOM | 1240 | CG2 | VAL | A | 160 | 4.097  | 52.814 | 46.314 | 1.00 | 32.12  |
| ATOM | 1241 | N   | SER | A | 161 | 2.132  | 53.967 | 43.760 | 1.00 | 29.81  |
| ATOM | 1242 | CA  | SER | A | 161 | 2.249  | 55.323 | 43.202 | 1.00 | 29.33  |
| ATOM | 1243 | C   | SER | A | 161 | 2.558  | 56.310 | 44.299 | 1.00 | 30.68  |
| ATOM | 1244 | O   | SER | A | 161 | 1.840  | 56.364 | 45.299 | 1.00 | 32.33  |
| ATOM | 1245 | CB  | SER | A | 161 | 0.963  | 55.756 | 42.514 | 1.00 | 32.12  |
| ATOM | 1246 | OG  | SER | A | 161 | 1.074  | 57.091 | 42.092 | 1.00 | 36.30  |
| ATOM | 1247 | N   | VAL | A | 162 | 3.614  | 57.073 | 44.115 | 1.00 | 24.51  |
| ATOM | 1248 | CA  | VAL | A | 162 | 3.968  | 58.033 | 45.125 | 1.00 | 25.24  |
| ATOM | 1249 | C   | VAL | A | 162 | 4.187  | 59.371 | 44.477 | 1.00 | 37.10  |
| ATOM | 1250 | O   | VAL | A | 162 | 4.359  | 59.438 | 43.257 | 1.00 | 36.28  |
| ATOM | 1251 | CB  | VAL | A | 162 | 5.284  | 57.657 | 45.821 | 1.00 | 25.44  |
| ATOM | 1252 | CG1 | VAL | A | 162 | 5.213  | 56.287 | 46.487 | 1.00 | 24.46  |
| ATOM | 1253 | CG2 | VAL | A | 162 | 6.429  | 57.684 | 44.831 | 1.00 | 24.47  |
| ATOM | 1254 | N   | PRO | A | 163 | 4.203  | 60.416 | 45.312 | 1.00 | 31.09  |
| ATOM | 1255 | CA  | PRO | A | 163 | 4.476  | 61.733 | 44.805 | 1.00 | 31.84  |
| ATOM | 1256 | C   | PRO | A | 163 | 5.792  | 61.640 | 44.040 | 1.00 | 31.38  |
| ATOM | 1257 | O   | PRO | A | 163 | 6.821  | 61.177 | 44.545 | 1.00 | 30.83  |
| ATOM | 1258 | CB  | PRO | A | 163 | 4.545  | 62.640 | 46.047 | 1.00 | 33.90  |
| ATOM | 1259 | CG  | PRO | A | 163 | 3.818  | 61.891 | 47.158 | 1.00 | 36.16  |
| ATOM | 1260 | CD  | PRO | A | 163 | 3.635  | 60.458 | 46.680 | 1.00 | 29.11  |
| ATOM | 1261 | N   | LYS | A | 164 | 5.738  | 62.040 | 42.789 | 1.00 | 30.95  |
| ATOM | 1262 | CA  | LYS | A | 164 | 6.875  | 61.950 | 41.891 | 1.00 | 30.90  |
| ATOM | 1263 | C   | LYS | A | 164 | 8.223  | 62.361 | 42.405 | 1.00 | 32.87  |
| ATOM | 1264 | O   | LYS | A | 164 | 9.249  | 61.973 | 41.850 | 1.00 | 29.98  |
| ATOM | 1265 | CB  | LYS | A | 164 | 6.614  | 62.525 | 40.525 | 1.00 | 38.69  |
| ATOM | 1266 | CG  | LYS | A | 164 | 5.381  | 63.405 | 40.464 | 1.00 | 60.47  |
| ATOM | 1267 | CD  | LYS | A | 164 | 5.608  | 64.642 | 39.612 | 1.00 | 87.95  |
| ATOM | 1268 | CE  | LYS | A | 164 | 6.869  | 64.557 | 38.757 | 1.00 | 94.83  |
| ATOM | 1269 | NZ  | LYS | A | 164 | 7.762  | 65.712 | 38.926 | 1.00 | 100.00 |
| ATOM | 1270 | N   | GLU | A | 165 | 8.253  | 63.168 | 43.445 | 1.00 | 32.55  |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 1271 | CA  | GLU | A | 165 | 9.540  | 63.587 | 43.946 | 1.00 | 33.95 |
| ATOM | 1272 | C   | GLU | A | 165 | 10.107 | 62.617 | 44.949 | 1.00 | 36.46 |
| ATOM | 1273 | O   | GLU | A | 165 | 11.245 | 62.742 | 45.348 | 1.00 | 36.58 |
| ATOM | 1274 | CB  | GLU | A | 165 | 9.510  | 65.006 | 44.540 | 1.00 | 37.35 |
| ATOM | 1275 | CG  | GLU | A | 165 | 8.599  | 65.165 | 45.784 | 1.00 | 53.54 |
| ATOM | 1276 | CD  | GLU | A | 165 | 7.138  | 65.409 | 45.480 | 1.00 | 77.59 |
| ATOM | 1277 | OE1 | GLU | A | 165 | 6.598  | 65.114 | 44.421 | 1.00 | 44.13 |
| ATOM | 1278 | OE2 | GLU | A | 165 | 6.512  | 65.959 | 46.494 | 1.00 | 78.66 |
| ATOM | 1279 | N   | LEU | A | 166 | 9.314  | 61.641 | 45.318 | 1.00 | 33.08 |
| ATOM | 1280 | CA  | LEU | A | 166 | 9.772  | 60.695 | 46.299 | 1.00 | 33.49 |
| ATOM | 1281 | C   | LEU | A | 166 | 10.068 | 59.321 | 45.734 | 1.00 | 40.05 |
| ATOM | 1282 | O   | LEU | A | 166 | 9.578  | 58.987 | 44.646 | 1.00 | 41.96 |
| ATOM | 1283 | CB  | LEU | A | 166 | 8.727  | 60.596 | 47.423 | 1.00 | 31.45 |
| ATOM | 1284 | CG  | LEU | A | 166 | 8.352  | 61.938 | 48.020 | 1.00 | 29.81 |
| ATOM | 1285 | CD1 | LEU | A | 166 | 7.242  | 61.711 | 49.041 | 1.00 | 27.01 |
| ATOM | 1286 | CD2 | LEU | A | 166 | 9.598  | 62.582 | 48.632 | 1.00 | 21.37 |
| ATOM | 1287 | N   | VAL | A | 167 | 10.874 | 58.544 | 46.500 | 1.00 | 30.67 |
| ATOM | 1288 | CA  | VAL | A | 167 | 11.238 | 57.178 | 46.138 | 1.00 | 29.31 |
| ATOM | 1289 | C   | VAL | A | 167 | 10.478 | 56.157 | 46.996 | 1.00 | 35.64 |
| ATOM | 1290 | O   | VAL | A | 167 | 10.216 | 56.385 | 48.183 | 1.00 | 32.65 |
| ATOM | 1291 | CB  | VAL | A | 167 | 12.721 | 56.904 | 46.304 | 1.00 | 30.60 |
| ATOM | 1292 | CG1 | VAL | A | 167 | 13.000 | 55.483 | 45.849 | 1.00 | 29.30 |
| ATOM | 1293 | CG2 | VAL | A | 167 | 13.562 | 57.880 | 45.521 | 1.00 | 31.04 |
| ATOM | 1294 | N   | ALA | A | 168 | 10.132 | 55.017 | 46.400 | 1.00 | 33.01 |
| ATOM | 1295 | CA  | ALA | A | 168 | 9.453  | 53.943 | 47.115 | 1.00 | 29.38 |
| ATOM | 1296 | C   | ALA | A | 168 | 10.289 | 52.685 | 46.978 | 1.00 | 36.90 |
| ATOM | 1297 | O   | ALA | A | 168 | 10.786 | 52.362 | 45.875 | 1.00 | 37.97 |
| ATOM | 1298 | CB  | ALA | A | 168 | 8.046  | 53.694 | 46.637 | 1.00 | 28.00 |
| ATOM | 1299 | N   | LEU | A | 169 | 10.482 | 51.997 | 48.110 | 1.00 | 28.52 |
| ATOM | 1300 | CA  | LEU | A | 169 | 11.256 | 50.769 | 48.139 | 1.00 | 24.26 |
| ATOM | 1301 | C   | LEU | A | 169 | 10.464 | 49.738 | 48.879 | 1.00 | 27.24 |
| ATOM | 1302 | O   | LEU | A | 169 | 9.694  | 50.071 | 49.786 | 1.00 | 25.74 |
| ATOM | 1303 | CB  | LEU | A | 169 | 12.615 | 50.908 | 48.841 | 1.00 | 24.31 |
| ATOM | 1304 | CG  | LEU | A | 169 | 13.525 | 51.974 | 48.250 | 1.00 | 28.56 |
| ATOM | 1305 | CD1 | LEU | A | 169 | 14.739 | 52.181 | 49.173 | 1.00 | 27.05 |
| ATOM | 1306 | CD2 | LEU | A | 169 | 13.993 | 51.550 | 46.852 | 1.00 | 27.25 |
| ATOM | 1307 | N   | MET | A | 170 | 10.649 | 48.480 | 48.486 | 1.00 | 26.02 |
| ATOM | 1308 | CA  | MET | A | 170 | 9.952  | 47.392 | 49.144 | 1.00 | 23.03 |
| ATOM | 1309 | C   | MET | A | 170 | 10.856 | 46.224 | 49.455 | 1.00 | 18.57 |
| ATOM | 1310 | O   | MET | A | 170 | 12.033 | 46.212 | 49.085 | 1.00 | 20.77 |
| ATOM | 1311 | CB  | MET | A | 170 | 8.712  | 46.943 | 48.371 | 1.00 | 24.60 |
| ATOM | 1312 | CG  | MET | A | 170 | 7.654  | 47.979 | 48.535 | 1.00 | 25.34 |
| ATOM | 1313 | SD  | MET | A | 170 | 6.105  | 47.419 | 47.869 | 1.00 | 28.58 |
| ATOM | 1314 | CE  | MET | A | 170 | 5.380  | 46.463 | 49.232 | 1.00 | 24.66 |
| ATOM | 1315 | N   | SER | A | 171 | 10.298 | 45.244 | 50.173 | 1.00 | 17.78 |
| ATOM | 1316 | CA  | SER | A | 171 | 11.062 | 44.069 | 50.482 | 1.00 | 16.80 |
| ATOM | 1317 | C   | SER | A | 171 | 10.905 | 43.128 | 49.265 | 1.00 | 26.03 |
| ATOM | 1318 | O   | SER | A | 171 | 10.389 | 42.018 | 49.344 | 1.00 | 25.31 |
| ATOM | 1319 | CB  | SER | A | 171 | 10.527 | 43.436 | 51.748 | 1.00 | 17.00 |
| ATOM | 1320 | OG  | SER | A | 171 | 9.130  | 43.207 | 51.625 | 1.00 | 20.17 |
| ATOM | 1321 | N   | ALA | A | 172 | 11.298 | 43.612 | 48.095 | 1.00 | 26.60 |
| ATOM | 1322 | CA  | ALA | A | 172 | 11.154 | 42.849 | 46.875 | 1.00 | 25.77 |
| ATOM | 1323 | C   | ALA | A | 172 | 12.153 | 43.339 | 45.860 | 1.00 | 32.28 |
| ATOM | 1324 | O   | ALA | A | 172 | 12.897 | 44.299 | 46.114 | 1.00 | 26.87 |
| ATOM | 1325 | CB  | ALA | A | 172 | 9.762  | 43.083 | 46.332 | 1.00 | 25.21 |
| ATOM | 1326 | N   | ILE | A | 173 | 12.180 | 42.678 | 44.700 | 1.00 | 30.44 |
| ATOM | 1327 | CA  | ILE | A | 173 | 13.107 | 43.110 | 43.661 | 1.00 | 29.54 |
| ATOM | 1328 | C   | ILE | A | 173 | 12.510 | 44.319 | 42.959 | 1.00 | 30.78 |



|      |      |     |     |   |     |        |        |        |      |        |
|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
| ATOM | 1329 | O   | ILE | A | 173 | 11.331 | 44.315 | 42.583 | 1.00 | 29.32  |
| ATOM | 1330 | CB  | ILE | A | 173 | 13.479 | 41.997 | 42.661 | 1.00 | 31.06  |
| ATOM | 1331 | CG1 | ILE | A | 173 | 14.210 | 40.874 | 43.388 | 1.00 | 28.42  |
| ATOM | 1332 | CG2 | ILE | A | 173 | 14.431 | 42.563 | 41.617 | 1.00 | 32.58  |
| ATOM | 1333 | CD1 | ILE | A | 173 | 15.604 | 41.286 | 43.851 | 1.00 | 33.22  |
| ATOM | 1334 | N   | ARG | A | 174 | 13.328 | 45.356 | 42.834 | 1.00 | 31.92  |
| ATOM | 1335 | CA  | ARG | A | 174 | 12.906 | 46.595 | 42.197 | 1.00 | 33.87  |
| ATOM | 1336 | C   | ARG | A | 174 | 12.582 | 46.236 | 40.785 | 1.00 | 39.44  |
| ATOM | 1337 | O   | ARG | A | 174 | 13.467 | 45.775 | 40.091 | 1.00 | 34.80  |
| ATOM | 1338 | CB  | ARG | A | 174 | 14.004 | 47.669 | 42.218 | 1.00 | 35.31  |
| ATOM | 1339 | CG  | ARG | A | 174 | 14.186 | 48.368 | 43.579 | 1.00 | 42.88  |
| ATOM | 1340 | CD  | ARG | A | 174 | 15.229 | 49.492 | 43.608 | 1.00 | 39.93  |
| ATOM | 1341 | NE  | ARG | A | 174 | 16.516 | 49.129 | 43.013 | 1.00 | 59.20  |
| ATOM | 1342 | CZ  | ARG | A | 174 | 17.329 | 49.992 | 42.407 | 1.00 | 92.36  |
| ATOM | 1343 | NH1 | ARG | A | 174 | 17.032 | 51.288 | 42.284 | 1.00 | 100.00 |
| ATOM | 1344 | NH2 | ARG | A | 174 | 18.474 | 49.542 | 41.901 | 1.00 | 84.94  |
| ATOM | 1345 | N   | ASP | A | 175 | 11.324 | 46.397 | 40.406 | 1.00 | 44.29  |
| ATOM | 1346 | CA  | ASP | A | 175 | 10.850 | 46.070 | 39.076 | 1.00 | 48.46  |
| ATOM | 1347 | C   | ASP | A | 175 | 10.987 | 47.236 | 38.107 | 1.00 | 61.94  |
| ATOM | 1348 | O   | ASP | A | 175 | 11.709 | 47.177 | 37.124 | 1.00 | 69.21  |
| ATOM | 1349 | CB  | ASP | A | 175 | 9.401  | 45.553 | 39.111 | 1.00 | 52.28  |
| ATOM | 1350 | CG  | ASP | A | 175 | 9.079  | 44.536 | 38.041 | 1.00 | 76.56  |
| ATOM | 1351 | OD1 | ASP | A | 175 | 9.926  | 44.028 | 37.313 | 1.00 | 76.21  |
| ATOM | 1352 | OD2 | ASP | A | 175 | 7.788  | 44.270 | 37.964 | 1.00 | 85.33  |
| ATOM | 1353 | N   | GLY | A | 176 | 10.293 | 48.309 | 38.369 | 1.00 | 59.49  |
| ATOM | 1354 | CA  | GLY | A | 176 | 10.405 | 49.442 | 37.489 | 1.00 | 59.25  |
| ATOM | 1355 | C   | GLY | A | 176 | 9.723  | 50.662 | 38.055 | 1.00 | 62.28  |
| ATOM | 1356 | O   | GLY | A | 176 | 8.958  | 50.585 | 39.026 | 1.00 | 61.93  |
| ATOM | 1357 | N   | GLU | A | 177 | 10.028 | 51.784 | 37.418 | 1.00 | 56.86  |
| ATOM | 1358 | CA  | GLU | A | 177 | 9.473  | 53.070 | 37.772 | 1.00 | 56.20  |
| ATOM | 1359 | C   | GLU | A | 177 | 9.128  | 53.804 | 36.495 | 1.00 | 66.31  |
| ATOM | 1360 | O   | GLU | A | 177 | 9.865  | 53.745 | 35.499 | 1.00 | 67.90  |
| ATOM | 1361 | CB  | GLU | A | 177 | 10.411 | 53.926 | 38.645 | 1.00 | 55.46  |
| ATOM | 1362 | CG  | GLU | A | 177 | 11.304 | 54.835 | 37.783 | 1.00 | 54.29  |
| ATOM | 1363 | CD  | GLU | A | 177 | 11.996 | 55.940 | 38.534 | 1.00 | 73.05  |
| ATOM | 1364 | OE1 | GLU | A | 177 | 11.471 | 57.005 | 38.805 | 1.00 | 66.34  |
| ATOM | 1365 | OE2 | GLU | A | 177 | 13.242 | 55.657 | 38.817 | 1.00 | 54.79  |
| ATOM | 1366 | N   | THR | A | 178 | 7.997  | 54.483 | 36.541 | 1.00 | 63.56  |
| ATOM | 1367 | CA  | THR | A | 178 | 7.496  | 55.245 | 35.419 | 1.00 | 63.49  |
| ATOM | 1368 | C   | THR | A | 178 | 6.534  | 56.305 | 35.923 | 1.00 | 64.39  |
| ATOM | 1369 | O   | THR | A | 178 | 6.338  | 56.452 | 37.118 | 1.00 | 65.55  |
| ATOM | 1370 | CB  | THR | A | 178 | 6.737  | 54.290 | 34.479 | 1.00 | 79.55  |
| ATOM | 1371 | OG1 | THR | A | 178 | 6.206  | 55.012 | 33.    |      |        |



|      |      |     |     |   |     |        |        |        |      |        |
|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
| ATOM | 1387 | OD2 | ASP | A | 180 | -0.383 | 57.463 | 39.973 | 1.00 | 47.57  |
| ATOM | 1388 | N   | PRO | A | 181 | -0.243 | 57.280 | 35.296 | 1.00 | 69.44  |
| ATOM | 1389 | CA  | PRO | A | 181 | -0.950 | 57.955 | 34.234 | 1.00 | 72.53  |
| ATOM | 1390 | C   | PRO | A | 181 | -2.382 | 58.272 | 34.587 | 1.00 | 82.99  |
| ATOM | 1391 | O   | PRO | A | 181 | -3.231 | 58.459 | 33.717 | 1.00 | 84.95  |
| ATOM | 1392 | CB  | PRO | A | 181 | -0.829 | 57.076 | 32.987 | 1.00 | 74.39  |
| ATOM | 1393 | CG  | PRO | A | 181 | 0.153  | 55.954 | 33.319 | 1.00 | 77.89  |
| ATOM | 1394 | CD  | PRO | A | 181 | 0.458  | 56.057 | 34.810 | 1.00 | 71.93  |
| ATOM | 1395 | N   | GLU | A | 182 | -2.632 | 58.382 | 35.887 | 1.00 | 83.47  |
| ATOM | 1396 | CA  | GLU | A | 182 | -3.961 | 58.676 | 36.386 | 1.00 | 86.24  |
| ATOM | 1397 | C   | GLU | A | 182 | -4.259 | 60.167 | 36.436 | 1.00 | 98.16  |
| ATOM | 1398 | O   | GLU | A | 182 | -4.003 | 60.882 | 35.460 | 1.00 | 100.00 |
| ATOM | 1399 | CB  | GLU | A | 182 | -4.278 | 57.994 | 37.726 | 1.00 | 87.28  |
| ATOM | 1400 | CG  | GLU | A | 182 | -5.779 | 57.681 | 37.863 | 1.00 | 90.17  |
| ATOM | 1401 | CD  | GLU | A | 182 | -6.257 | 56.682 | 36.842 | 1.00 | 100.00 |
| ATOM | 1402 | OE1 | GLU | A | 182 | -6.233 | 56.882 | 35.637 | 1.00 | 100.00 |
| ATOM | 1403 | OE2 | GLU | A | 182 | -6.718 | 55.578 | 37.385 | 1.00 | 100.00 |
| ATOM | 1404 | N   | ASP | A | 183 | -4.767 | 60.640 | 37.598 | 1.00 | 96.59  |
| ATOM | 1405 | CA  | ASP | A | 183 | -5.124 | 62.060 | 37.848 | 1.00 | 97.69  |
| ATOM | 1406 | C   | ASP | A | 183 | -4.078 | 62.809 | 38.721 | 1.00 | 100.00 |
| ATOM | 1407 | O   | ASP | A | 183 | -4.439 | 63.829 | 39.375 | 1.00 | 100.00 |
| ATOM | 1408 | CB  | ASP | A | 183 | -6.477 | 62.127 | 38.653 | 1.00 | 99.62  |
| ATOM | 1409 | CG  | ASP | A | 183 | -7.712 | 61.432 | 38.090 | 1.00 | 100.00 |
| ATOM | 1410 | OD1 | ASP | A | 183 | -8.310 | 60.544 | 38.680 | 1.00 | 100.00 |
| ATOM | 1411 | OD2 | ASP | A | 183 | -8.091 | 61.903 | 36.918 | 1.00 | 100.00 |
| ATOM | 1412 | N   | PRO | A | 184 | -2.797 | 62.341 | 38.750 | 1.00 | 95.70  |
| ATOM | 1413 | CA  | PRO | A | 184 | -1.734 | 62.796 | 39.641 | 1.00 | 94.16  |
| ATOM | 1414 | C   | PRO | A | 184 | -0.516 | 63.593 | 39.206 | 1.00 | 96.46  |
| ATOM | 1415 | O   | PRO | A | 184 | -0.294 | 63.958 | 38.050 | 1.00 | 99.66  |
| ATOM | 1416 | CB  | PRO | A | 184 | -0.980 | 61.479 | 39.654 | 1.00 | 95.77  |
| ATOM | 1417 | CG  | PRO | A | 184 | -0.835 | 61.166 | 38.163 | 1.00 | 99.25  |
| ATOM | 1418 | CD  | PRO | A | 184 | -2.085 | 61.763 | 37.565 | 1.00 | 94.91  |
| ATOM | 1419 | N   | SER | A | 185 | 0.318  | 63.703 | 40.258 | 1.00 | 86.69  |
| ATOM | 1420 | CA  | SER | A | 185 | 1.658  | 64.262 | 40.362 | 1.00 | 82.33  |
| ATOM | 1421 | C   | SER | A | 185 | 2.434  | 63.253 | 41.219 | 1.00 | 77.73  |
| ATOM | 1422 | O   | SER | A | 185 | 3.198  | 63.570 | 42.144 | 1.00 | 79.49  |
| ATOM | 1423 | CB  | SER | A | 185 | 1.710  | 65.661 | 40.921 | 1.00 | 85.04  |
| ATOM | 1424 | OG  | SER | A | 185 | 2.756  | 66.349 | 40.263 | 1.00 | 97.98  |
| ATOM | 1425 | N   | ARG | A | 186 | 2.121  | 61.994 | 40.856 | 1.00 | 62.61  |
| ATOM | 1426 | CA  | ARG | A | 186 | 2.591  | 60.741 | 41.404 | 1.00 | 55.55  |
| ATOM | 1427 | C   | ARG | A | 186 | 3.444  | 59.990 | 40.366 | 1.00 | 56.85  |
| ATOM | 1428 | O   | ARG | A | 186 | 3.354  | 60.216 | 39.158 | 1.00 | 56.42  |
| ATOM | 1429 | CB  | ARG | A | 186 | 1.388  | 59.859 | 41.742 | 1.00 | 41.52  |
|      |      |     |     |   |     |        |        |        |      |        |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 1445 | N   | ILE | A | 188 | 5.006  | 55.832 | 39.620 | 1.00 | 46.34 |
| ATOM | 1446 | CA  | ILE | A | 188 | 4.732  | 54.438 | 39.963 | 1.00 | 43.89 |
| ATOM | 1447 | C   | ILE | A | 188 | 5.884  | 53.438 | 40.044 | 1.00 | 45.27 |
| ATOM | 1448 | O   | ILE | A | 188 | 6.596  | 53.147 | 39.068 | 1.00 | 42.03 |
| ATOM | 1449 | CB  | ILE | A | 188 | 3.357  | 53.861 | 39.782 | 1.00 | 46.49 |
| ATOM | 1450 | CG1 | ILE | A | 188 | 3.571  | 52.427 | 39.378 | 1.00 | 46.61 |
| ATOM | 1451 | CG2 | ILE | A | 188 | 2.528  | 54.603 | 38.744 | 1.00 | 45.69 |
| ATOM | 1452 | CD1 | ILE | A | 188 | 2.888  | 51.492 | 40.354 | 1.00 | 66.60 |
| ATOM | 1453 | N   | TYR | A | 189 | 6.055  | 52.933 | 41.277 | 1.00 | 39.79 |
| ATOM | 1454 | CA  | TYR | A | 189 | 7.108  | 52.024 | 41.630 | 1.00 | 36.01 |
| ATOM | 1455 | C   | TYR | A | 189 | 6.634  | 50.615 | 41.665 | 1.00 | 36.02 |
| ATOM | 1456 | O   | TYR | A | 189 | 5.632  | 50.291 | 42.321 | 1.00 | 36.41 |
| ATOM | 1457 | CB  | TYR | A | 189 | 7.766  | 52.446 | 42.952 | 1.00 | 37.07 |
| ATOM | 1458 | CG  | TYR | A | 189 | 8.644  | 53.677 | 42.783 | 1.00 | 36.77 |
| ATOM | 1459 | CD1 | TYR | A | 189 | 9.904  | 53.567 | 42.197 | 1.00 | 39.01 |
| ATOM | 1460 | CD2 | TYR | A | 189 | 8.216  | 54.942 | 43.193 | 1.00 | 34.62 |
| ATOM | 1461 | CE1 | TYR | A | 189 | 10.733 | 54.675 | 42.029 | 1.00 | 41.28 |
| ATOM | 1462 | CE2 | TYR | A | 189 | 9.023  | 56.067 | 43.031 | 1.00 | 33.53 |
| ATOM | 1463 | CZ  | TYR | A | 189 | 10.279 | 55.927 | 42.441 | 1.00 | 44.38 |
| ATOM | 1464 | OH  | TYR | A | 189 | 11.084 | 57.022 | 42.277 | 1.00 | 44.92 |
| ATOM | 1465 | N   | LYS | A | 190 | 7.395  | 49.801 | 40.929 | 1.00 | 35.47 |
| ATOM | 1466 | CA  | LYS | A | 190 | 7.125  | 48.373 | 40.772 | 1.00 | 36.67 |
| ATOM | 1467 | C   | LYS | A | 190 | 8.131  | 47.441 | 41.475 | 1.00 | 32.16 |
| ATOM | 1468 | O   | LYS | A | 190 | 9.337  | 47.667 | 41.471 | 1.00 | 30.99 |
| ATOM | 1469 | CB  | LYS | A | 190 | 6.872  | 47.992 | 39.310 | 1.00 | 39.45 |
| ATOM | 1470 | CG  | LYS | A | 190 | 5.457  | 48.328 | 38.833 | 1.00 | 44.38 |
| ATOM | 1471 | CD  | LYS | A | 190 | 5.417  | 49.126 | 37.539 | 1.00 | 56.65 |
| ATOM | 1472 | CE  | LYS | A | 190 | 5.539  | 48.274 | 36.282 | 1.00 | 73.04 |
| ATOM | 1473 | NZ  | LYS | A | 190 | 6.686  | 48.658 | 35.433 | 1.00 | 92.77 |
| ATOM | 1474 | N   | PHE | A | 191 | 7.592  | 46.380 | 42.076 | 1.00 | 27.93 |
| ATOM | 1475 | CA  | PHE | A | 191 | 8.393  | 45.421 | 42.812 | 1.00 | 25.63 |
| ATOM | 1476 | C   | PHE | A | 191 | 7.916  | 43.986 | 42.679 | 1.00 | 25.33 |
| ATOM | 1477 | O   | PHE | A | 191 | 6.708  | 43.667 | 42.633 | 1.00 | 24.55 |
| ATOM | 1478 | CB  | PHE | A | 191 | 8.281  | 45.779 | 44.306 | 1.00 | 27.49 |
| ATOM | 1479 | CG  | PHE | A | 191 | 8.548  | 47.238 | 44.618 | 1.00 | 26.47 |
| ATOM | 1480 | CD1 | PHE | A | 191 | 9.838  | 47.668 | 44.922 | 1.00 | 27.21 |
| ATOM | 1481 | CD2 | PHE | A | 191 | 7.508  | 48.167 | 44.619 | 1.00 | 27.67 |
| ATOM | 1482 | CE1 | PHE | A | 191 | 10.086 | 49.004 | 45.223 | 1.00 | 28.50 |
| ATOM | 1483 | CE2 | PHE | A | 191 | 7.739  | 49.510 | 44.909 | 1.00 | 29.86 |
| ATOM | 1484 | CZ  | PHE | A | 191 | 9.038  | 49.923 | 45.205 | 1.00 | 28.47 |
| ATOM | 1485 | N   | ILE | A | 192 | 8.868  | 43.076 | 42.700 | 1.00 | 26.53 |
| ATOM | 1486 | CA  | ILE | A | 192 | 8.485  | 41.669 | 42.616 | 1.00 | 30.09 |
| ATOM | 1487 | C   | ILE | A | 192 | 9.228  | 40.779 | 43.609 | 1.00 |       |



|      |      |     |           |        |        |        |      |       |
|------|------|-----|-----------|--------|--------|--------|------|-------|
| ATOM | 1503 | CA  | LYS A 194 | 9.486  | 35.548 | 43.842 | 1.00 | 26.30 |
| ATOM | 1504 | C   | LYS A 194 | 9.677  | 34.457 | 44.943 | 1.00 | 33.55 |
| ATOM | 1505 | O   | LYS A 194 | 9.254  | 33.305 | 44.759 | 1.00 | 33.23 |
| ATOM | 1506 | CB  | LYS A 194 | 10.379 | 35.289 | 42.612 | 1.00 | 26.74 |
| ATOM | 1507 | CG  | LYS A 194 | 9.722  | 35.609 | 41.258 | 1.00 | 39.96 |
| ATOM | 1508 | CD  | LYS A 194 | 10.697 | 36.137 | 40.199 | 1.00 | 47.00 |
| ATOM | 1509 | CE  | LYS A 194 | 10.182 | 36.110 | 38.751 | 1.00 | 59.13 |
| ATOM | 1510 | NZ  | LYS A 194 | 11.226 | 35.798 | 37.746 | 1.00 | 54.07 |
| ATOM | 1511 | N   | VAL A 195 | 10.332 | 34.795 | 46.076 | 1.00 | 25.61 |
| ATOM | 1512 | CA  | VAL A 195 | 10.542 | 33.829 | 47.155 | 1.00 | 23.02 |
| ATOM | 1513 | C   | VAL A 195 | 9.385  | 33.947 | 48.108 | 1.00 | 27.87 |
| ATOM | 1514 | O   | VAL A 195 | 9.099  | 35.029 | 48.566 | 1.00 | 29.77 |
| ATOM | 1515 | CB  | VAL A 195 | 11.833 | 34.049 | 47.930 | 1.00 | 22.42 |
| ATOM | 1516 | CG1 | VAL A 195 | 11.997 | 32.891 | 48.881 | 1.00 | 22.09 |
| ATOM | 1517 | CG2 | VAL A 195 | 13.057 | 34.101 | 47.027 | 1.00 | 21.83 |
| ATOM | 1518 | N   | PRO A 196 | 8.687  | 32.867 | 48.391 | 1.00 | 24.28 |
| ATOM | 1519 | CA  | PRO A 196 | 7.572  | 32.955 | 49.297 | 1.00 | 22.68 |
| ATOM | 1520 | C   | PRO A 196 | 8.042  | 33.362 | 50.704 | 1.00 | 27.58 |
| ATOM | 1521 | O   | PRO A 196 | 9.027  | 32.837 | 51.244 | 1.00 | 25.38 |
| ATOM | 1522 | CB  | PRO A 196 | 6.886  | 31.588 | 49.301 | 1.00 | 24.52 |
| ATOM | 1523 | CG  | PRO A 196 | 7.686  | 30.674 | 48.397 | 1.00 | 28.81 |
| ATOM | 1524 | CD  | PRO A 196 | 8.822  | 31.497 | 47.831 | 1.00 | 24.64 |
| ATOM | 1525 | N   | ILE A 197 | 7.339  | 34.328 | 51.287 | 1.00 | 22.20 |
| ATOM | 1526 | CA  | ILE A 197 | 7.713  | 34.810 | 52.578 | 1.00 | 19.62 |
| ATOM | 1527 | C   | ILE A 197 | 6.498  | 35.005 | 53.418 | 1.00 | 24.85 |
| ATOM | 1528 | O   | ILE A 197 | 5.391  | 35.163 | 52.919 | 1.00 | 20.49 |
| ATOM | 1529 | CB  | ILE A 197 | 8.307  | 36.176 | 52.383 | 1.00 | 21.90 |
| ATOM | 1530 | CG1 | ILE A 197 | 7.317  | 36.930 | 51.510 | 1.00 | 23.26 |
| ATOM | 1531 | CG2 | ILE A 197 | 9.662  | 36.133 | 51.681 | 1.00 | 22.57 |
| ATOM | 1532 | CD1 | ILE A 197 | 7.442  | 38.455 | 51.650 | 1.00 | 28.64 |
| ATOM | 1533 | N   | PRO A 198 | 6.725  | 35.020 | 54.727 | 1.00 | 22.95 |
| ATOM | 1534 | CA  | PRO A 198 | 5.660  | 35.263 | 55.686 | 1.00 | 20.55 |
| ATOM | 1535 | C   | PRO A 198 | 5.308  | 36.740 | 55.535 | 1.00 | 24.13 |
| ATOM | 1536 | O   | PRO A 198 | 6.192  | 37.511 | 55.197 | 1.00 | 24.11 |
| ATOM | 1537 | CB  | PRO A 198 | 6.286  | 35.001 | 57.046 | 1.00 | 20.69 |
| ATOM | 1538 | CG  | PRO A 198 | 7.782  | 34.882 | 56.848 | 1.00 | 24.39 |
| ATOM | 1539 | CD  | PRO A 198 | 8.046  | 34.830 | 55.359 | 1.00 | 21.23 |
| ATOM | 1540 | N   | CYS A 199 | 4.029  | 37.129 | 55.721 | 1.00 | 22.42 |
| ATOM | 1541 | CA  | CYS A 199 | 3.597  | 38.521 | 55.530 | 1.00 | 23.29 |
| ATOM | 1542 | C   | CYS A 199 | 4.310  | 39.559 | 56.408 | 1.00 | 27.78 |
| ATOM | 1543 | O   | CYS A 199 | 4.378  | 40.752 | 56.060 | 1.00 | 25.00 |
| ATOM | 1544 | CB  | CYS A 199 | 2.079  | 38.691 | 55.499 | 1.00 | 24.93 |
| ATOM | 1545 | SG  | CYS A 199 | 1.319  | 38.281 | 57.082 | 1.00 | 31.80 |
| ATOM | 1546 | N   | TYR A 200 | 4.880  | 39.106 | 57.542 | 1.00 | 21.98 |
| ATOM | 1547 | CA  | TYR A 200 | 5.590  | 40.062 | 58.390 | 1.00 | 19.50 |
| ATOM | 1548 | C   | TYR A 200 | 6.812  | 40.615 | 57.730 | 1.00 | 21.02 |
| ATOM | 1549 | O   | TYR A 200 | 7.392  | 41.585 | 58.195 | 1.00 | 19.63 |



|      |      |     |           |        |        |        |      |       |
|------|------|-----|-----------|--------|--------|--------|------|-------|
| ATOM | 1561 | O   | LEU A 201 | 8.840  | 41.791 | 53.934 | 1.00 | 21.66 |
| ATOM | 1562 | CB  | LEU A 201 | 9.177  | 39.235 | 55.381 | 1.00 | 16.83 |
| ATOM | 1563 | CG  | LEU A 201 | 9.786  | 38.370 | 56.484 | 1.00 | 18.02 |
| ATOM | 1564 | CD1 | LEU A 201 | 10.522 | 37.230 | 55.803 | 1.00 | 19.59 |
| ATOM | 1565 | CD2 | LEU A 201 | 10.792 | 39.169 | 57.271 | 1.00 | 14.71 |
| ATOM | 1566 | N   | ILE A 202 | 6.733  | 41.795 | 54.687 | 1.00 | 21.47 |
| ATOM | 1567 | CA  | ILE A 202 | 6.283  | 42.764 | 53.681 | 1.00 | 21.65 |
| ATOM | 1568 | C   | ILE A 202 | 6.660  | 44.150 | 54.204 | 1.00 | 26.05 |
| ATOM | 1569 | O   | ILE A 202 | 6.278  | 44.529 | 55.321 | 1.00 | 23.20 |
| ATOM | 1570 | CB  | ILE A 202 | 4.780  | 42.726 | 53.439 | 1.00 | 24.75 |
| ATOM | 1571 | CG1 | ILE A 202 | 4.373  | 41.403 | 52.800 | 1.00 | 23.39 |
| ATOM | 1572 | CG2 | ILE A 202 | 4.437  | 43.900 | 52.512 | 1.00 | 28.50 |
| ATOM | 1573 | CD1 | ILE A 202 | 2.864  | 41.172 | 52.728 | 1.00 | 31.47 |
| ATOM | 1574 | N   | ALA A 203 | 7.427  | 44.894 | 53.431 | 1.00 | 19.73 |
| ATOM | 1575 | CA  | ALA A 203 | 7.855  | 46.204 | 53.877 | 1.00 | 22.65 |
| ATOM | 1576 | C   | ALA A 203 | 7.838  | 47.244 | 52.757 | 1.00 | 25.87 |
| ATOM | 1577 | O   | ALA A 203 | 8.068  | 46.955 | 51.585 | 1.00 | 23.99 |
| ATOM | 1578 | CB  | ALA A 203 | 9.258  | 46.153 | 54.511 | 1.00 | 23.47 |
| ATOM | 1579 | N   | LEU A 204 | 7.607  | 48.474 | 53.198 | 1.00 | 19.67 |
| ATOM | 1580 | CA  | LEU A 204 | 7.538  | 49.632 | 52.347 | 1.00 | 18.99 |
| ATOM | 1581 | C   | LEU A 204 | 8.093  | 50.857 | 53.051 | 1.00 | 23.68 |
| ATOM | 1582 | O   | LEU A 204 | 7.893  | 51.074 | 54.253 | 1.00 | 21.71 |
| ATOM | 1583 | CB  | LEU A 204 | 6.061  | 49.879 | 51.935 | 1.00 | 18.01 |
| ATOM | 1584 | CG  | LEU A 204 | 5.814  | 51.197 | 51.176 | 1.00 | 23.52 |
| ATOM | 1585 | CD1 | LEU A 204 | 6.230  | 51.125 | 49.697 | 1.00 | 21.41 |
| ATOM | 1586 | CD2 | LEU A 204 | 4.345  | 51.563 | 51.285 | 1.00 | 21.73 |
| ATOM | 1587 | N   | VAL A 205 | 8.786  | 51.648 | 52.258 | 1.00 | 22.72 |
| ATOM | 1588 | CA  | VAL A 205 | 9.348  | 52.893 | 52.693 | 1.00 | 21.77 |
| ATOM | 1589 | C   | VAL A 205 | 9.200  | 53.882 | 51.559 | 1.00 | 26.12 |
| ATOM | 1590 | O   | VAL A 205 | 9.508  | 53.568 | 50.406 | 1.00 | 24.95 |
| ATOM | 1591 | CB  | VAL A 205 | 10.812 | 52.781 | 53.027 | 1.00 | 25.95 |
| ATOM | 1592 | CG1 | VAL A 205 | 11.521 | 52.212 | 51.803 | 1.00 | 26.40 |
| ATOM | 1593 | CG2 | VAL A 205 | 11.340 | 54.192 | 53.317 | 1.00 | 27.95 |
| ATOM | 1594 | N   | VAL A 206 | 8.732  | 55.066 | 51.880 | 1.00 | 20.44 |



|      |      |     |     |   |     |        |        |        |      |        |
|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
| ATOM | 1595 | CA  | VAL | A | 206 | 8.576  | 56.105 | 50.858 | 1.00 | 21.96  |
| ATOM | 1596 | C   | VAL | A | 206 | 9.265  | 57.379 | 51.324 | 1.00 | 28.78  |
| ATOM | 1597 | O   | VAL | A | 206 | 9.008  | 57.824 | 52.447 | 1.00 | 28.18  |
| ATOM | 1598 | CB  | VAL | A | 206 | 7.109  | 56.389 | 50.536 | 1.00 | 23.95  |
| ATOM | 1599 | CG1 | VAL | A | 206 | 7.004  | 57.493 | 49.488 | 1.00 | 25.31  |
| ATOM | 1600 | CG2 | VAL | A | 206 | 6.442  | 55.118 | 50.037 | 1.00 | 23.22  |
| ATOM | 1601 | N   | GLY | A | 207 | 10.139 | 57.941 | 50.498 | 1.00 | 25.04  |
| ATOM | 1602 | CA  | GLY | A | 207 | 10.797 | 59.159 | 50.914 | 1.00 | 26.83  |
| ATOM | 1603 | C   | GLY | A | 207 | 11.775 | 59.691 | 49.899 | 1.00 | 28.05  |
| ATOM | 1604 | O   | GLY | A | 207 | 11.859 | 59.189 | 48.780 | 1.00 | 29.36  |
| ATOM | 1605 | N   | ALA | A | 208 | 12.502 | 60.711 | 50.346 | 1.00 | 26.69  |
| ATOM | 1606 | CA  | ALA | A | 208 | 13.536 | 61.410 | 49.578 | 1.00 | 29.20  |
| ATOM | 1607 | C   | ALA | A | 208 | 14.846 | 60.654 | 49.687 | 1.00 | 31.12  |
| ATOM | 1608 | O   | ALA | A | 208 | 15.796 | 61.079 | 50.353 | 1.00 | 29.49  |
| ATOM | 1609 | CB  | ALA | A | 208 | 13.684 | 62.841 | 50.104 | 1.00 | 30.49  |
| ATOM | 1610 | N   | LEU | A | 209 | 14.856 | 59.514 | 49.014 | 1.00 | 28.20  |
| ATOM | 1611 | CA  | LEU | A | 209 | 15.963 | 58.592 | 49.036 | 1.00 | 28.72  |
| ATOM | 1612 | C   | LEU | A | 209 | 17.012 | 58.709 | 47.959 | 1.00 | 38.13  |
| ATOM | 1613 | O   | LEU | A | 209 | 16.751 | 58.982 | 46.799 | 1.00 | 42.08  |
| ATOM | 1614 | CB  | LEU | A | 209 | 15.453 | 57.135 | 49.139 | 1.00 | 26.94  |
| ATOM | 1615 | CG  | LEU | A | 209 | 14.440 | 57.028 | 50.261 | 1.00 | 31.37  |
| ATOM | 1616 | CD1 | LEU | A | 209 | 13.636 | 55.747 | 50.154 | 1.00 | 33.38  |
| ATOM | 1617 | CD2 | LEU | A | 209 | 15.188 | 57.065 | 51.581 | 1.00 | 30.28  |
| ATOM | 1618 | N   | GLU | A | 210 | 18.212 | 58.437 | 48.418 | 1.00 | 32.71  |
| ATOM | 1619 | CA  | GLU | A | 210 | 19.403 | 58.405 | 47.650 | 1.00 | 31.96  |
| ATOM | 1620 | C   | GLU | A | 210 | 20.080 | 57.121 | 48.033 | 1.00 | 37.22  |
| ATOM | 1621 | O   | GLU | A | 210 | 19.837 | 56.606 | 49.126 | 1.00 | 34.80  |
| ATOM | 1622 | CB  | GLU | A | 210 | 20.295 | 59.616 | 47.927 | 1.00 | 32.87  |
| ATOM | 1623 | CG  | GLU | A | 210 | 19.833 | 60.822 | 47.107 | 1.00 | 44.60  |
| ATOM | 1624 | CD  | GLU | A | 210 | 20.785 | 61.953 | 47.229 | 1.00 | 82.71  |
| ATOM | 1625 | OE1 | GLU | A | 210 | 21.889 | 61.829 | 47.732 | 1.00 | 73.15  |
| ATOM | 1626 | OE2 | GLU | A | 210 | 20.295 | 63.072 | 46.753 | 1.00 | 100.00 |
| ATOM | 1627 | N   | SER | A | 211 | 20.877 | 56.614 | 47.105 | 1.00 | 35.47  |
| ATOM | 1628 | CA  | SER | A | 211 | 21.581 | 55.369 | 47.253 | 1.00 | 34.32  |
| ATOM | 1629 | C   | SER | A | 211 | 23.045 | 55.490 | 46.911 | 1.00 | 39.68  |
| ATOM | 1630 | O   | SER | A | 211 | 23.478 | 56.390 | 46.219 | 1.00 | 45.50  |
| ATOM | 1631 | CB  | SER | A | 211 | 20.922 | 54.288 | 46.378 | 1.00 | 38.13  |
| ATOM | 1632 | OG  | SER | A | 211 | 21.157 | 54.494 | 44.982 | 1.00 | 40.31  |
| ATOM | 1633 | N   | ARG | A | 212 | 23.819 | 54.569 | 47.381 | 1.00 | 30.48  |
| ATOM | 1634 | CA  | ARG | A | 212 | 25.210 | 54.541 | 47.065 | 1.00 | 29.53  |
| ATOM | 1635 | C   | ARG | A | 212 | 25.507 | 53.063 | 46.924 | 1.00 | 35.68  |
| ATOM | 1636 | O   | ARG | A | 212 | 25.101 | 52.275 | 47.774 | 1.00 | 35.76  |
| ATOM | 1637 | CB  | ARG | A | 212 | 26.043 | 55.203 | 48.147 | 1.00 | 32.65  |
| ATOM | 1638 | CG  | ARG | A | 212 | 27.304 | 55.851 | 47.600 | 1.00 | 56.68  |
| ATOM | 1639 | CD  | ARG | A | 212 | 27.035 | 57.020 | 46.647 | 1.00 | 73.87  |
| ATOM | 1640 | NE  | ARG | A | 212 | 26.884 | 58.345 | 47.270 | 1.00 | 68.27  |
| ATOM | 1641 | CZ  | ARG | A | 212 | 25.863 | 59.200 | 47.037 | 1.00 | 85.21  |
| ATOM | 1642 | NH1 | ARG | A | 212 | 24.847 | 58.918 | 46.205 | 1.00 | 40.25  |
| ATOM | 1643 | NH2 | ARG | A | 212 | 25.860 | 60.383 | 47.666 | 1.00 | 87.08  |
| ATOM | 1644 | N   | GLN | A | 213 | 26.137 | 52.645 | 45.851 | 1.00 | 28.72  |
| ATOM | 1645 | CA  | GLN | A | 213 | 26.400 | 51.238 | 45.722 | 1.00 | 29.18  |
| ATOM | 1646 | C   | GLN | A | 213 | 27.663 | 50.855 | 46.475 | 1.00 | 34.58  |
| ATOM | 1647 | O   | GLN | A | 213 | 28.716 | 51.434 | 46.220 | 1.00 | 36.75  |
| ATOM | 1648 | CB  | GLN | A | 213 | 26.487 | 50.838 | 44.251 | 1.00 | 30.88  |
| ATOM | 1649 | CG  | GLN | A | 213 | 26.268 | 49.331 | 44.057 | 1.00 | 42.35  |
| ATOM | 1650 | CD  | GLN | A | 213 | 26.898 | 48.872 | 42.780 | 1.00 | 61.33  |
| ATOM | 1651 | OE1 | GLN | A | 213 | 27.585 | 47.845 | 42.754 | 1.00 | 55.13  |
| ATOM | 1652 | NE2 | GLN | A | 213 | 26.679 | 49.658 | 41.724 | 1.00 | 65.90  |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 1653 | N   | ILE | A | 214 | 27.553 | 49.880 | 47.413 | 1.00 | 28.70 |
| ATOM | 1654 | CA  | ILE | A | 214 | 28.697 | 49.455 | 48.202 | 1.00 | 25.96 |
| ATOM | 1655 | C   | ILE | A | 214 | 29.065 | 48.017 | 47.970 | 1.00 | 29.90 |
| ATOM | 1656 | O   | ILE | A | 214 | 29.925 | 47.468 | 48.651 | 1.00 | 30.32 |
| ATOM | 1657 | CB  | ILE | A | 214 | 28.495 | 49.694 | 49.685 | 1.00 | 27.31 |
| ATOM | 1658 | CG1 | ILE | A | 214 | 27.292 | 48.905 | 50.161 | 1.00 | 27.09 |
| ATOM | 1659 | CG2 | ILE | A | 214 | 28.191 | 51.159 | 49.913 | 1.00 | 28.84 |
| ATOM | 1660 | CD1 | ILE | A | 214 | 27.092 | 49.010 | 51.667 | 1.00 | 24.71 |
| ATOM | 1661 | N   | GLY | A | 215 | 28.393 | 47.400 | 47.020 | 1.00 | 27.12 |
| ATOM | 1662 | CA  | GLY | A | 215 | 28.660 | 45.988 | 46.697 | 1.00 | 28.78 |
| ATOM | 1663 | C   | GLY | A | 215 | 27.921 | 45.548 | 45.441 | 1.00 | 33.65 |
| ATOM | 1664 | O   | GLY | A | 215 | 26.945 | 46.193 | 45.060 | 1.00 | 37.47 |
| ATOM | 1665 | N   | PRO | A | 216 | 28.375 | 44.451 | 44.813 | 1.00 | 31.69 |
| ATOM | 1666 | CA  | PRO | A | 216 | 27.777 | 43.940 | 43.596 | 1.00 | 31.17 |
| ATOM | 1667 | C   | PRO | A | 216 | 26.293 | 43.725 | 43.726 | 1.00 | 34.01 |
| ATOM | 1668 | O   | PRO | A | 216 | 25.549 | 43.848 | 42.762 | 1.00 | 37.18 |
| ATOM | 1669 | CB  | PRO | A | 216 | 28.441 | 42.615 | 43.281 | 1.00 | 32.10 |
| ATOM | 1670 | CG  | PRO | A | 216 | 29.337 | 42.292 | 44.453 | 1.00 | 36.37 |
| ATOM | 1671 | CD  | PRO | A | 216 | 29.255 | 43.453 | 45.426 | 1.00 | 31.79 |
| ATOM | 1672 | N   | ARG | A | 217 | 25.856 | 43.409 | 44.918 | 1.00 | 23.91 |
| ATOM | 1673 | CA  | ARG | A | 217 | 24.440 | 43.187 | 45.108 | 1.00 | 24.07 |
| ATOM | 1674 | C   | ARG | A | 217 | 23.912 | 44.068 | 46.225 | 1.00 | 31.39 |
| ATOM | 1675 | O   | ARG | A | 217 | 22.863 | 43.803 | 46.826 | 1.00 | 30.65 |
| ATOM | 1676 | CB  | ARG | A | 217 | 24.150 | 41.717 | 45.382 | 1.00 | 26.69 |
| ATOM | 1677 | CG  | ARG | A | 217 | 25.327 | 40.950 | 46.011 | 1.00 | 38.32 |
| ATOM | 1678 | CD  | ARG | A | 217 | 24.955 | 39.534 | 46.476 | 1.00 | 26.86 |
| ATOM | 1679 | NE  | ARG | A | 217 | 26.022 | 38.855 | 47.227 | 1.00 | 27.11 |
| ATOM | 1680 | CZ  | ARG | A | 217 | 26.038 | 37.550 | 47.494 | 1.00 | 36.87 |
| ATOM | 1681 | NH1 | ARG | A | 217 | 25.070 | 36.732 | 47.082 | 1.00 | 29.90 |
| ATOM | 1682 | NH2 | ARG | A | 217 | 27.053 | 37.051 | 48.188 | 1.00 | 34.57 |
| ATOM | 1683 | N   | THR | A | 218 | 24.669 | 45.121 | 46.503 | 1.00 | 24.92 |
| ATOM | 1684 | CA  | THR | A | 218 | 24.283 | 45.994 | 47.561 | 1.00 | 24.28 |
| ATOM | 1685 | C   | THR | A | 218 | 24.407 | 47.495 | 47.295 | 1.00 | 33.11 |
| ATOM | 1686 | O   | THR | A | 218 | 25.462 | 48.009 | 46.938 | 1.00 | 32.08 |
| ATOM | 1687 | CB  | THR | A | 218 | 25.099 | 45.694 | 48.842 | 1.00 | 25.29 |
| ATOM | 1688 | OG1 | THR | A | 218 | 25.110 | 44.320 | 49.114 | 1.00 | 29.80 |
| ATOM | 1689 | CG2 | THR | A | 218 | 24.550 | 46.489 | 50.042 | 1.00 | 19.82 |
| ATOM | 1690 | N   | LEU | A | 219 | 23.294 | 48.168 | 47.577 | 1.00 | 30.26 |
| ATOM | 1691 | CA  | LEU | A | 219 | 23.138 | 49.593 | 47.547 | 1.00 | 30.69 |
| ATOM | 1692 | C   | LEU | A | 219 | 22.755 | 50.013 | 48.964 | 1.00 | 35.22 |
| ATOM | 1693 | O   | LEU | A | 219 | 22.157 | 49.227 | 49.717 | 1.00 | 33.12 |
| ATOM | 1694 | CB  | LEU | A | 219 | 21.963 | 49.979 | 46.668 | 1.00 | 31.36 |
| ATOM | 1695 | CG  | LEU | A | 219 | 22.394 | 50.547 |        |      |       |



|      |      |     |     |   |     |        |        |        |      |        |
|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
| ATOM | 1711 | CD1 | TRP | A | 221 | 18.817 | 51.334 | 48.993 | 1.00 | 29.93  |
| ATOM | 1712 | CD2 | TRP | A | 221 | 17.949 | 53.044 | 47.866 | 1.00 | 28.26  |
| ATOM | 1713 | NE1 | TRP | A | 221 | 18.686 | 50.951 | 47.687 | 1.00 | 28.94  |
| ATOM | 1714 | CE2 | TRP | A | 221 | 18.158 | 51.980 | 46.969 | 1.00 | 31.62  |
| ATOM | 1715 | CE3 | TRP | A | 221 | 17.404 | 54.250 | 47.397 | 1.00 | 29.01  |
| ATOM | 1716 | CZ2 | TRP | A | 221 | 17.841 | 52.093 | 45.616 | 1.00 | 31.03  |
| ATOM | 1717 | CZ3 | TRP | A | 221 | 17.093 | 54.351 | 46.059 | 1.00 | 29.62  |
| ATOM | 1718 | CH2 | TRP | A | 221 | 17.319 | 53.284 | 45.177 | 1.00 | 29.13  |
| ATOM | 1719 | N   | SER | A | 222 | 19.277 | 56.047 | 51.843 | 1.00 | 27.55  |
| ATOM | 1720 | CA  | SER | A | 222 | 19.002 | 56.889 | 52.991 | 1.00 | 28.55  |
| ATOM | 1721 | C   | SER | A | 222 | 18.770 | 58.317 | 52.528 | 1.00 | 37.74  |
| ATOM | 1722 | O   | SER | A | 222 | 18.945 | 58.649 | 51.341 | 1.00 | 36.03  |
| ATOM | 1723 | CB  | SER | A | 222 | 20.012 | 56.786 | 54.145 | 1.00 | 25.75  |
| ATOM | 1724 | OG  | SER | A | 222 | 21.148 | 57.591 | 53.888 | 1.00 | 32.66  |
| ATOM | 1725 | N   | GLU | A | 223 | 18.423 | 59.174 | 53.446 | 1.00 | 30.01  |
| ATOM | 1726 | CA  | GLU | A | 223 | 18.297 | 60.498 | 52.991 | 1.00 | 28.87  |
| ATOM | 1727 | C   | GLU | A | 223 | 19.713 | 60.922 | 52.600 | 1.00 | 34.38  |
| ATOM | 1728 | O   | GLU | A | 223 | 20.731 | 60.373 | 53.065 | 1.00 | 29.90  |
| ATOM | 1729 | CB  | GLU | A | 223 | 17.732 | 61.411 | 54.081 | 1.00 | 29.74  |
| ATOM | 1730 | CG  | GLU | A | 223 | 16.184 | 61.485 | 54.050 | 1.00 | 36.16  |
| ATOM | 1731 | CD  | GLU | A | 223 | 15.638 | 62.563 | 54.967 | 1.00 | 64.35  |
| ATOM | 1732 | OE1 | GLU | A | 223 | 15.376 | 63.690 | 54.583 | 1.00 | 29.91  |
| ATOM | 1733 | OE2 | GLU | A | 223 | 15.465 | 62.169 | 56.219 | 1.00 | 46.08  |
| ATOM | 1734 | N   | LYS | A | 224 | 19.765 | 61.913 | 51.722 | 1.00 | 33.08  |
| ATOM | 1735 | CA  | LYS | A | 224 | 21.006 | 62.468 | 51.231 | 1.00 | 32.76  |
| ATOM | 1736 | C   | LYS | A | 224 | 22.054 | 62.700 | 52.335 | 1.00 | 31.27  |
| ATOM | 1737 | O   | LYS | A | 224 | 23.257 | 62.463 | 52.195 | 1.00 | 29.06  |
| ATOM | 1738 | CB  | LYS | A | 224 | 20.655 | 63.795 | 50.547 | 1.00 | 36.11  |
| ATOM | 1739 | CG  | LYS | A | 224 | 21.845 | 64.676 | 50.237 | 1.00 | 70.27  |
| ATOM | 1740 | CD  | LYS | A | 224 | 21.558 | 65.670 | 49.112 | 1.00 | 95.60  |
| ATOM | 1741 | CE  | LYS | A | 224 | 22.191 | 65.293 | 47.774 | 1.00 | 100.00 |
| ATOM | 1742 | NZ  | LYS | A | 224 | 21.521 | 65.907 | 46.613 | 1.00 | 100.00 |
| ATOM | 1743 | N   | GLU | A | 225 | 21.595 | 63.197 | 53.449 | 1.00 | 27.65  |
| ATOM | 1744 | CA  | GLU | A | 225 | 22.466 | 63.510 | 54.560 | 1.00 | 30.22  |
| ATOM | 1745 | C   | GLU | A | 225 | 23.173 | 62.347 | 55.232 | 1.00 | 34.65  |
| ATOM | 1746 | O   | GLU | A | 225 | 24.093 | 62.573 | 56.012 | 1.00 | 32.34  |
| ATOM | 1747 | CB  | GLU | A | 225 | 21.691 | 64.278 | 55.645 | 1.00 | 31.76  |
| ATOM | 1748 | CG  | GLU | A | 225 | 21.276 | 65.694 | 55.193 | 1.00 | 42.16  |
| ATOM | 1749 | CD  | GLU | A | 225 | 19.998 | 65.742 | 54.394 | 1.00 | 65.10  |
| ATOM | 1750 | OE1 | GLU | A | 225 | 19.395 | 66.779 | 54.196 | 1.00 | 45.97  |
| ATOM | 1751 | OE2 | GLU | A | 225 | 19.599 | 64.571 | 53.932 | 1.00 | 45.63  |
| ATOM | 1752 | N   | GLN | A | 226 | 22.752 | 61.120 | 54.973 | 1.00 | 33.60  |
| ATOM | 1753 | CA  |     |   |     |        |        |        |      |        |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 1769 | CA  | GLU | A | 228 | 28.291 | 58.805 | 52.664 | 1.00 | 32.15 |
| ATOM | 1770 | C   | GLU | A | 228 | 28.689 | 57.981 | 53.870 | 1.00 | 36.09 |
| ATOM | 1771 | O   | GLU | A | 228 | 29.400 | 56.995 | 53.735 | 1.00 | 33.16 |
| ATOM | 1772 | CB  | GLU | A | 228 | 29.031 | 60.144 | 52.584 | 1.00 | 34.27 |
| ATOM | 1773 | CG  | GLU | A | 228 | 28.993 | 60.704 | 51.145 | 1.00 | 69.42 |
| ATOM | 1774 | CD  | GLU | A | 228 | 29.273 | 59.645 | 50.108 | 1.00 | 98.31 |
| ATOM | 1775 | OE1 | GLU | A | 228 | 30.359 | 59.101 | 50.017 | 1.00 | 94.37 |
| ATOM | 1776 | OE2 | GLU | A | 228 | 28.238 | 59.362 | 49.343 | 1.00 | 74.62 |
| ATOM | 1777 | N   | LYS | A | 229 | 28.202 | 58.433 | 55.044 | 1.00 | 33.36 |
| ATOM | 1778 | CA  | LYS | A | 229 | 28.419 | 57.808 | 56.348 | 1.00 | 30.47 |
| ATOM | 1779 | C   | LYS | A | 229 | 27.897 | 56.378 | 56.335 | 1.00 | 27.55 |
| ATOM | 1780 | O   | LYS | A | 229 | 28.545 | 55.446 | 56.780 | 1.00 | 28.17 |
| ATOM | 1781 | CB  | LYS | A | 229 | 27.650 | 58.563 | 57.415 | 1.00 | 31.12 |
| ATOM | 1782 | CG  | LYS | A | 229 | 28.477 | 59.545 | 58.209 | 1.00 | 55.25 |
| ATOM | 1783 | CD  | LYS | A | 229 | 27.835 | 59.871 | 59.550 | 1.00 | 64.16 |
| ATOM | 1784 | CE  | LYS | A | 229 | 28.242 | 58.886 | 60.642 | 1.00 | 63.01 |
| ATOM | 1785 | NZ  | LYS | A | 229 | 29.694 | 58.883 | 60.899 | 1.00 | 59.75 |
| ATOM | 1786 | N   | SER | A | 230 | 26.700 | 56.201 | 55.838 | 1.00 | 22.45 |
| ATOM | 1787 | CA  | SER | A | 230 | 26.198 | 54.864 | 55.798 | 1.00 | 22.46 |
| ATOM | 1788 | C   | SER | A | 230 | 27.053 | 54.034 | 54.872 | 1.00 | 27.74 |
| ATOM | 1789 | O   | SER | A | 230 | 27.407 | 52.894 | 55.125 | 1.00 | 24.67 |
| ATOM | 1790 | CB  | SER | A | 230 | 24.806 | 54.881 | 55.263 | 1.00 | 23.20 |
| ATOM | 1791 | OG  | SER | A | 230 | 24.116 | 55.844 | 56.004 | 1.00 | 35.82 |
| ATOM | 1792 | N   | ALA | A | 231 | 27.371 | 54.626 | 53.759 | 1.00 | 26.64 |
| ATOM | 1793 | CA  | ALA | A | 231 | 28.173 | 53.922 | 52.803 | 1.00 | 28.26 |
| ATOM | 1794 | C   | ALA | A | 231 | 29.482 | 53.482 | 53.455 | 1.00 | 35.74 |
| ATOM | 1795 | O   | ALA | A | 231 | 30.004 | 52.384 | 53.260 | 1.00 | 38.85 |
| ATOM | 1796 | CB  | ALA | A | 231 | 28.386 | 54.807 | 51.575 | 1.00 | 28.68 |
| ATOM | 1797 | N   | TYR | A | 232 | 30.040 | 54.332 | 54.280 | 1.00 | 28.97 |
| ATOM | 1798 | CA  | TYR | A | 232 | 31.288 | 53.956 | 54.919 | 1.00 | 25.66 |
| ATOM | 1799 | C   | TYR | A | 232 | 31.106 | 52.830 | 55.956 | 1.00 | 26.63 |
| ATOM | 1800 | O   | TYR | A | 232 | 31.764 | 51.786 | 55.952 | 1.00 | 24.11 |
| ATOM | 1801 | CB  | TYR | A | 232 | 31.878 | 55.221 | 55.590 | 1.00 | 26.53 |
| ATOM | 1802 | CG  | TYR | A | 232 | 33.048 | 54.883 | 56.450 | 1.00 | 30.29 |
| ATOM | 1803 | CD1 | TYR | A | 232 | 34.327 | 54.751 | 55.908 | 1.00 | 30.47 |
| ATOM | 1804 | CD2 | TYR | A | 232 | 32.868 | 54.647 | 57.812 | 1.00 | 34.13 |
| ATOM | 1805 | CE1 | TYR | A | 232 | 35.417 | 54.417 | 56.707 | 1.00 | 26.95 |
| ATOM | 1806 | CE2 | TYR | A | 232 | 33.943 | 54.289 | 58.629 | 1.00 | 34.94 |
| ATOM | 1807 | CZ  | TYR | A | 232 | 35.214 | 54.187 | 58.066 | 1.00 | 44.35 |
| ATOM | 1808 | OH  | TYR | A | 232 | 36.267 | 53.838 | 58.863 | 1.00 | 56.64 |
| ATOM | 1809 | N   | GLU | A | 233 | 30.179 | 53.101 | 56.854 | 1.00 | 26.62 |
| ATOM | 1810 | CA  | GLU | A | 233 | 29.848 | 52.255 | 57.979 | 1.00 | 27.40 |
| ATOM | 1811 | C   | GLU | A | 233 |        |        |        |      |       |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 1827 | CE2 | PHE | A | 234 | 24.461 | 51.411 | 57.526 | 1.00 | 28.00 |
| ATOM | 1828 | CZ  | PHE | A | 234 | 24.697 | 51.113 | 58.869 | 1.00 | 23.00 |
| ATOM | 1829 | N   | SER | A | 235 | 30.508 | 49.151 | 54.883 | 1.00 | 27.12 |
| ATOM | 1830 | CA  | SER | A | 235 | 31.342 | 48.689 | 53.787 | 1.00 | 25.76 |
| ATOM | 1831 | C   | SER | A | 235 | 31.469 | 47.166 | 53.731 | 1.00 | 31.87 |
| ATOM | 1832 | O   | SER | A | 235 | 31.329 | 46.571 | 52.658 | 1.00 | 31.51 |
| ATOM | 1833 | CB  | SER | A | 235 | 32.706 | 49.348 | 53.801 | 1.00 | 23.97 |
| ATOM | 1834 | OG  | SER | A | 235 | 33.403 | 49.017 | 54.987 | 1.00 | 31.36 |
| ATOM | 1835 | N   | GLU | A | 236 | 31.715 | 46.554 | 54.905 | 1.00 | 24.57 |
| ATOM | 1836 | CA  | GLU | A | 236 | 31.883 | 45.120 | 55.032 | 1.00 | 23.90 |
| ATOM | 1837 | C   | GLU | A | 236 | 30.683 | 44.241 | 54.687 | 1.00 | 26.57 |
| ATOM | 1838 | O   | GLU | A | 236 | 30.735 | 43.032 | 54.900 | 1.00 | 26.86 |
| ATOM | 1839 | CB  | GLU | A | 236 | 32.348 | 44.786 | 56.440 | 1.00 | 25.38 |
| ATOM | 1840 | CG  | GLU | A | 236 | 33.520 | 45.662 | 56.873 | 1.00 | 34.31 |
| ATOM | 1841 | CD  | GLU | A | 236 | 33.663 | 45.666 | 58.366 | 1.00 | 73.76 |
| ATOM | 1842 | OE1 | GLU | A | 236 | 32.739 | 45.910 | 59.133 | 1.00 | 40.32 |
| ATOM | 1843 | OE2 | GLU | A | 236 | 34.876 | 45.354 | 58.750 | 1.00 | 83.10 |
| ATOM | 1844 | N   | THR | A | 237 | 29.610 | 44.828 | 54.150 | 1.00 | 20.07 |
| ATOM | 1845 | CA  | THR | A | 237 | 28.437 | 44.060 | 53.819 | 1.00 | 18.84 |
| ATOM | 1846 | C   | THR | A | 237 | 28.713 | 42.900 | 52.887 | 1.00 | 27.55 |
| ATOM | 1847 | O   | THR | A | 237 | 28.342 | 41.774 | 53.189 | 1.00 | 29.80 |
| ATOM | 1848 | CB  | THR | A | 237 | 27.276 | 44.944 | 53.339 | 1.00 | 27.61 |
| ATOM | 1849 | OG1 | THR | A | 237 | 26.930 | 45.851 | 54.347 | 1.00 | 26.27 |
| ATOM | 1850 | CG2 | THR | A | 237 | 26.046 | 44.143 | 52.933 | 1.00 | 20.18 |
| ATOM | 1851 | N   | GLU | A | 238 | 29.346 | 43.140 | 51.747 | 1.00 | 24.98 |
| ATOM | 1852 | CA  | GLU | A | 238 | 29.605 | 42.022 | 50.840 | 1.00 | 25.71 |
| ATOM | 1853 | C   | GLU | A | 238 | 30.408 | 40.914 | 51.463 | 1.00 | 27.50 |
| ATOM | 1854 | O   | GLU | A | 238 | 30.091 | 39.740 | 51.324 | 1.00 | 30.32 |
| ATOM | 1855 | CB  | GLU | A | 238 | 30.169 | 42.373 | 49.467 | 1.00 | 27.51 |
| ATOM | 1856 | CG  | GLU | A | 238 | 30.292 | 41.101 | 48.580 | 1.00 | 31.12 |
| ATOM | 1857 | CD  | GLU | A | 238 | 29.006 | 40.489 | 48.048 | 1.00 | 29.47 |
| ATOM | 1858 | OE1 | GLU | A | 238 | 27.929 | 41.034 | 47.978 | 1.00 | 38.32 |
| ATOM | 1859 | OE2 | GLU | A | 238 | 29.179 | 39.289 | 47.615 | 1.00 | 42.12 |
| ATOM | 1860 | N   | SER | A | 239 | 31.452 | 41.269 | 52.164 | 1.00 | 21.93 |
| ATOM | 1861 | CA  | SER | A | 239 | 32.224 | 40.232 | 52.797 | 1.00 | 21.40 |
| ATOM | 1862 | C   | SER | A | 239 | 31.377 | 39.410 | 53.774 | 1.00 | 26.79 |
| ATOM | 1863 | O   | SER | A | 239 | 31.519 | 38.208 | 53.878 | 1.00 | 26.27 |
| ATOM | 1864 | CB  | SER | A | 239 | 33.430 | 40.788 | 53.514 | 1.00 | 24.31 |
| ATOM | 1865 | OG  | SER | A | 239 | 32.995 | 41.369 | 54.724 | 1.00 | 36.29 |
| ATOM | 1866 | N   | MET | A | 240 | 30.485 | 40.044 | 54.530 | 1.00 | 25.33 |
| ATOM | 1867 | CA  | MET | A | 240 | 29.664 | 39.280 | 55.453 | 1.00 | 21.61 |
| ATOM | 1868 | C   | MET | A | 240 | 28.750 | 38.383 | 54.688 | 1.00 | 26.18 |
| ATOM | 1869 | O   | MET | A | 240 | 28.580 |        |        |      |       |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 1885 | O   | LYS | A | 242 | 30.026 | 33.662 | 52.290 | 1.00 | 25.83 |
| ATOM | 1886 | CB  | LYS | A | 242 | 31.267 | 36.205 | 50.763 | 1.00 | 30.42 |
| ATOM | 1887 | CG  | LYS | A | 242 | 31.015 | 36.447 | 49.291 | 1.00 | 32.91 |
| ATOM | 1888 | CD  | LYS | A | 242 | 32.171 | 37.142 | 48.591 | 1.00 | 59.75 |
| ATOM | 1889 | CE  | LYS | A | 242 | 31.815 | 38.564 | 48.172 | 1.00 | 63.56 |
| ATOM | 1890 | NZ  | LYS | A | 242 | 32.262 | 38.944 | 46.821 | 1.00 | 60.62 |
| ATOM | 1891 | N   | ILE | A | 243 | 30.490 | 35.282 | 53.766 | 1.00 | 21.79 |
| ATOM | 1892 | CA  | ILE | A | 243 | 30.698 | 34.341 | 54.858 | 1.00 | 22.45 |
| ATOM | 1893 | C   | ILE | A | 243 | 29.405 | 33.594 | 55.138 | 1.00 | 24.79 |
| ATOM | 1894 | O   | ILE | A | 243 | 29.362 | 32.375 | 55.319 | 1.00 | 24.38 |
| ATOM | 1895 | CB  | ILE | A | 243 | 31.237 | 35.038 | 56.109 | 1.00 | 25.48 |
| ATOM | 1896 | CG1 | ILE | A | 243 | 32.592 | 35.666 | 55.815 | 1.00 | 27.23 |
| ATOM | 1897 | CG2 | ILE | A | 243 | 31.354 | 34.044 | 57.263 | 1.00 | 24.60 |
| ATOM | 1898 | CD1 | ILE | A | 243 | 33.202 | 36.392 | 57.016 | 1.00 | 24.23 |
| ATOM | 1899 | N   | ALA | A | 244 | 28.339 | 34.372 | 55.128 | 1.00 | 19.81 |
| ATOM | 1900 | CA  | ALA | A | 244 | 27.047 | 33.837 | 55.384 | 1.00 | 19.55 |
| ATOM | 1901 | C   | ALA | A | 244 | 26.690 | 32.721 | 54.413 | 1.00 | 27.11 |
| ATOM | 1902 | O   | ALA | A | 244 | 26.100 | 31.692 | 54.790 | 1.00 | 25.26 |
| ATOM | 1903 | CB  | ALA | A | 244 | 26.031 | 34.969 | 55.400 | 1.00 | 19.21 |
| ATOM | 1904 | N   | GLU | A | 245 | 27.066 | 32.933 | 53.146 | 1.00 | 27.29 |
| ATOM | 1905 | CA  | GLU | A | 245 | 26.761 | 31.949 | 52.111 | 1.00 | 25.68 |
| ATOM | 1906 | C   | GLU | A | 245 | 27.436 | 30.651 | 52.396 | 1.00 | 30.57 |
| ATOM | 1907 | O   | GLU | A | 245 | 26.869 | 29.580 | 52.183 | 1.00 | 30.82 |
| ATOM | 1908 | CB  | GLU | A | 245 | 27.084 | 32.415 | 50.691 | 1.00 | 25.71 |
| ATOM | 1909 | CG  | GLU | A | 245 | 25.914 | 33.199 | 50.106 | 1.00 | 31.03 |
| ATOM | 1910 | CD  | GLU | A | 245 | 26.225 | 33.838 | 48.794 | 1.00 | 38.47 |
| ATOM | 1911 | OE1 | GLU | A | 245 | 27.175 | 34.588 | 48.613 | 1.00 | 36.65 |
| ATOM | 1912 | OE2 | GLU | A | 245 | 25.353 | 33.507 | 47.876 | 1.00 | 42.50 |
| ATOM | 1913 | N   | ASP | A | 246 | 28.649 | 30.778 | 52.887 | 1.00 | 25.43 |
| ATOM | 1914 | CA  | ASP | A | 246 | 29.451 | 29.643 | 53.212 | 1.00 | 26.46 |
| ATOM | 1915 | C   | ASP | A | 246 | 28.875 | 28.913 | 54.410 | 1.00 | 31.36 |
| ATOM | 1916 | O   | ASP | A | 246 | 28.969 | 27.701 | 54.571 | 1.00 | 33.32 |
| ATOM | 1917 | CB  | ASP | A | 246 | 30.900 | 30.080 | 53.480 | 1.00 | 31.18 |
| ATOM | 1918 | CG  | ASP | A | 246 | 31.794 | 28.904 | 53.736 | 1.00 | 65.05 |
| ATOM | 1919 | OD1 | ASP | A | 246 | 32.175 | 28.171 | 52.842 | 1.00 | 74.67 |
| ATOM | 1920 | OD2 | ASP | A | 246 | 32.085 | 28.726 | 55.010 | 1.00 | 73.86 |
| ATOM | 1921 | N   | LEU | A | 247 | 28.253 | 29.651 | 55.267 | 1.00 | 24.37 |
| ATOM | 1922 | CA  | LEU | A | 247 | 27.713 | 29.020 | 56.425 | 1.00 | 24.71 |
| ATOM | 1923 | C   | LEU | A | 247 | 26.326 | 28.469 | 56.212 | 1.00 | 27.23 |
| ATOM | 1924 | O   | LEU | A | 247 | 26.025 | 27.388 | 56.709 | 1.00 | 29.85 |
| ATOM | 1925 | CB  | LEU | A | 247 | 27.715 | 29.984 | 57.653 | 1.00 | 25.90 |
| ATOM | 1926 | CG  | LEU | A | 247 | 29.069 | 30.647 | 57.905 | 1.00 | 28.01 |
| ATOM | 1927 | CD1 | LEU | A | 247 | 28.934 | 31.696 | 58.983 | 1.00 | 27.01 |
| ATOM | 1928 | CD2 | LEU | A | 247 | 30.051 | 29.603 | 58.370 | 1.00 | 30.42 |
| ATOM | 1929 | N   | GLY | A | 248 | 25.454 | 29.203 | 55.517 | 1.00 | 23.34 |
| ATOM | 1930 | CA  | GLY | A | 248 | 24.102 | 28.671 | 55.384 | 1.00 | 23.65 |
| ATOM | 1931 | C   | GLY | A | 248 | 23.720 | 28.204 | 53.993 | 1.00 | 27.51 |
| ATOM | 1932 | O   | GLY | A | 248 | 22.598 | 27.784 | 53.765 | 1.00 | 24.78 |
| ATOM | 1933 | N   | GLY | A | 249 | 24.635 | 28.283 | 53.047 | 1.00 | 23.68 |
| ATOM | 1934 | CA  | GLY | A | 249 | 24.250 | 27.882 | 51.729 | 1.00 | 23.61 |
| ATOM | 1935 | C   | GLY | A | 249 | 23.951 | 29.127 | 50.944 | 1.00 | 31.96 |
| ATOM | 1936 | O   | GLY | A | 249 | 23.996 | 30.204 | 51.471 | 1.00 | 30.39 |
| ATOM | 1937 | N   | PRO | A | 250 | 23.640 | 28.981 | 49.674 | 1.00 | 37.24 |
| ATOM | 1938 | CA  | PRO | A | 250 | 23.359 | 30.099 | 48.806 | 1.00 | 38.84 |
| ATOM | 1939 | C   | PRO | A | 250 | 22.317 | 31.103 | 49.290 | 1.00 | 37.99 |
| ATOM | 1940 | O   | PRO | A | 250 | 21.289 | 30.775 | 49.903 | 1.00 | 35.02 |
| ATOM | 1941 | CB  | PRO | A | 250 | 22.830 | 29.484 | 47.504 | 1.00 | 41.32 |
| ATOM | 1942 | CG  | PRO | A | 250 | 22.393 | 28.072 | 47.831 | 1.00 | 44.27 |



669220-072209

|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 1943 | CD  | PRO | A | 250 | 23.026 | 27.730 | 49.162 | 1.00 | 40.21 |
| ATOM | 1944 | N   | TYR | A | 251 | 22.616 | 32.351 | 48.956 | 1.00 | 31.18 |
| ATOM | 1945 | CA  | TYR | A | 251 | 21.758 | 33.456 | 49.230 | 1.00 | 26.41 |
| ATOM | 1946 | C   | TYR | A | 251 | 20.802 | 33.418 | 48.067 | 1.00 | 27.76 |
| ATOM | 1947 | O   | TYR | A | 251 | 21.234 | 33.528 | 46.926 | 1.00 | 27.95 |
| ATOM | 1948 | CB  | TYR | A | 251 | 22.601 | 34.723 | 49.143 | 1.00 | 25.32 |
| ATOM | 1949 | CG  | TYR | A | 251 | 21.787 | 35.954 | 49.397 | 1.00 | 28.06 |
| ATOM | 1950 | CD1 | TYR | A | 251 | 21.368 | 36.246 | 50.695 | 1.00 | 29.60 |
| ATOM | 1951 | CD2 | TYR | A | 251 | 21.437 | 36.831 | 48.367 | 1.00 | 27.85 |
| ATOM | 1952 | CE1 | TYR | A | 251 | 20.618 | 37.392 | 50.963 | 1.00 | 28.45 |
| ATOM | 1953 | CE2 | TYR | A | 251 | 20.687 | 37.982 | 48.616 | 1.00 | 27.14 |
| ATOM | 1954 | CZ  | TYR | A | 251 | 20.292 | 38.270 | 49.926 | 1.00 | 25.89 |
| ATOM | 1955 | OH  | TYR | A | 251 | 19.551 | 39.392 | 50.199 | 1.00 | 20.56 |
| ATOM | 1956 | N   | VAL | A | 252 | 19.519 | 33.243 | 48.328 | 1.00 | 24.99 |
| ATOM | 1957 | CA  | VAL | A | 252 | 18.535 | 33.115 | 47.251 | 1.00 | 25.59 |
| ATOM | 1958 | C   | VAL | A | 252 | 17.696 | 34.351 | 46.925 | 1.00 | 28.69 |
| ATOM | 1959 | O   | VAL | A | 252 | 16.868 | 34.320 | 46.014 | 1.00 | 25.00 |
| ATOM | 1960 | CB  | VAL | A | 252 | 17.562 | 31.979 | 47.627 | 1.00 | 30.01 |
| ATOM | 1961 | CG1 | VAL | A | 252 | 18.288 | 30.668 | 47.953 | 1.00 | 29.63 |
| ATOM | 1962 | CG2 | VAL | A | 252 | 16.646 | 32.391 | 48.789 | 1.00 | 29.32 |
| ATOM | 1963 | N   | TRP | A | 253 | 17.858 | 35.425 | 47.689 | 1.00 | 25.81 |
| ATOM | 1964 | CA  | TRP | A | 253 | 17.046 | 36.599 | 47.504 | 1.00 | 23.18 |
| ATOM | 1965 | C   | TRP | A | 253 | 17.432 | 37.542 | 46.388 | 1.00 | 28.15 |
| ATOM | 1966 | O   | TRP | A | 253 | 16.655 | 38.427 | 46.037 | 1.00 | 27.55 |
| ATOM | 1967 | CB  | TRP | A | 253 | 16.824 | 37.329 | 48.813 | 1.00 | 19.42 |
| ATOM | 1968 | CG  | TRP | A | 253 | 16.418 | 36.383 | 49.878 | 1.00 | 20.56 |
| ATOM | 1969 | CD1 | TRP | A | 253 | 17.256 | 35.687 | 50.673 | 1.00 | 22.97 |
| ATOM | 1970 | CD2 | TRP | A | 253 | 15.087 | 36.014 | 50.249 | 1.00 | 19.71 |
| ATOM | 1971 | NE1 | TRP | A | 253 | 16.525 | 34.902 | 51.541 | 1.00 | 22.22 |
| ATOM | 1972 | CE2 | TRP | A | 253 | 15.192 | 35.109 | 51.309 | 1.00 | 22.80 |
| ATOM | 1973 | CE3 | TRP | A | 253 | 13.829 | 36.398 | 49.817 | 1.00 | 21.50 |
| ATOM | 1974 | CZ2 | TRP | A | 253 | 14.063 | 34.577 | 51.925 | 1.00 | 23.69 |
| ATOM | 1975 | CZ3 | TRP | A | 253 | 12.709 | 35.878 | 50.412 | 1.00 | 24.31 |
| ATOM | 1976 | CH2 | TRP | A | 253 | 12.823 | 34.974 | 51.466 | 1.00 | 24.84 |
| ATOM | 1977 | N   | GLY | A | 254 | 18.625 | 37.367 | 45.843 | 1.00 | 25.04 |
| ATOM | 1978 | CA  | GLY | A | 254 | 19.102 | 38.192 | 44.739 | 1.00 | 26.11 |
| ATOM | 1979 | C   | GLY | A | 254 | 19.864 | 39.404 | 45.200 | 1.00 | 31.09 |
| ATOM | 1980 | O   | GLY | A | 254 | 21.098 | 39.431 | 45.258 | 1.00 | 34.73 |
| ATOM | 1981 | N   | GLN | A | 255 | 19.098 | 40.410 | 45.535 | 1.00 | 29.08 |
| ATOM | 1982 | CA  | GLN | A | 255 | 19.648 | 41.666 | 45.995 | 1.00 | 29.63 |
| ATOM | 1983 | C   | GLN | A | 255 | 19.728 | 41.712 | 47.507 | 1.00 | 29.64 |
| ATOM | 1984 | O   | GLN | A | 255 | 18.887 | 41.114 | 48.196 | 1.00 | 30.51 |
| ATOM | 1985 | CB  | GLN | A | 255 | 18.784 | 42.833 | 45.468 | 1.00 | 31.78 |
| ATOM | 1986 | CG  | GLN | A | 255 | 19.424 | 44.221 | 45.672 | 1.00 | 44.26 |
| ATOM | 1987 | CD  | GLN | A | 255 | 20.587 | 44.500 | 44.732 | 1.00 | 54.96 |
| ATOM | 1988 | OE1 | GLN | A | 255 | 21.252 | 45.543 | 44.825 | 1.00 | 36.97 |
| ATOM | 1989 | NE2 | GLN | A | 255 | 20.846 | 43.559 | 43.829 | 1.00 | 52.17 |
| ATOM | 1990 | N   | TYR | A | 256 | 20.763 | 42.399 | 47.992 | 1.00 | 27.13 |
| ATOM | 1991 | CA  | TYR | A | 256 | 20.978 | 42.641 | 49.402 | 1.00 | 25.23 |
| ATOM | 1992 | C   | TYR | A | 256 | 21.188 | 44.115 | 49.648 | 1.00 | 25.37 |
| ATOM | 1993 | O   | TYR | A | 256 | 22.317 | 44.554 | 49.816 | 1.00 | 25.89 |
| ATOM | 1994 | CB  | TYR | A | 256 | 22.034 | 41.819 | 50.137 | 1.00 | 25.95 |
| ATOM | 1995 | CG  | TYR | A | 256 | 21.872 | 42.059 | 51.629 | 1.00 | 24.48 |
| ATOM | 1996 | CD1 | TYR | A | 256 | 20.961 | 41.306 | 52.373 | 1.00 | 25.11 |
| ATOM | 1997 | CD2 | TYR | A | 256 | 22.604 | 43.053 | 52.281 | 1.00 | 24.57 |
| ATOM | 1998 | CB1 | TYR | A | 256 | 20.779 | 41.529 | 53.738 | 1.00 | 22.81 |
| ATOM | 1999 | CE2 | TYR | A | 256 | 22.423 | 43.302 | 53.640 | 1.00 | 23.52 |
| ATOM | 2000 | CZ  | TYR | A | 256 | 21.523 | 42.526 | 54.369 | 1.00 | 27.26 |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 2001 | OH  | TYR | A | 256 | 21.356 | 42.772 | 55.707 | 1.00 | 26.88 |
| ATOM | 2002 | N   | ASP | A | 257 | 20.080 | 44.863 | 49.634 | 1.00 | 22.34 |
| ATOM | 2003 | CA  | ASP | A | 257 | 20.118 | 46.288 | 49.871 | 1.00 | 19.26 |
| ATOM | 2004 | C   | ASP | A | 257 | 19.947 | 46.597 | 51.343 | 1.00 | 27.05 |
| ATOM | 2005 | O   | ASP | A | 257 | 19.324 | 45.823 | 52.093 | 1.00 | 26.42 |
| ATOM | 2006 | CB  | ASP | A | 257 | 19.064 | 47.071 | 49.069 | 1.00 | 19.63 |
| ATOM | 2007 | CG  | ASP | A | 257 | 19.470 | 47.325 | 47.621 | 1.00 | 38.29 |
| ATOM | 2008 | OD1 | ASP | A | 257 | 20.533 | 46.922 | 47.146 | 1.00 | 35.24 |
| ATOM | 2009 | OD2 | ASP | A | 257 | 18.557 | 47.994 | 46.914 | 1.00 | 33.46 |
| ATOM | 2010 | N   | LEU | A | 258 | 20.488 | 47.772 | 51.708 | 1.00 | 25.54 |
| ATOM | 2011 | CA  | LEU | A | 258 | 20.451 | 48.319 | 53.050 | 1.00 | 23.91 |
| ATOM | 2012 | C   | LEU | A | 258 | 19.752 | 49.651 | 53.020 | 1.00 | 27.43 |
| ATOM | 2013 | O   | LEU | A | 258 | 20.058 | 50.464 | 52.152 | 1.00 | 26.91 |
| ATOM | 2014 | CB  | LEU | A | 258 | 21.861 | 48.551 | 53.612 | 1.00 | 23.00 |
| ATOM | 2015 | CG  | LEU | A | 258 | 22.542 | 47.293 | 54.130 | 1.00 | 24.65 |
| ATOM | 2016 | CD1 | LEU | A | 258 | 23.897 | 47.652 | 54.753 | 1.00 | 21.61 |
| ATOM | 2017 | CD2 | LEU | A | 258 | 21.650 | 46.669 | 55.192 | 1.00 | 27.74 |
| ATOM | 2018 | N   | LEU | A | 259 | 18.824 | 49.843 | 53.974 | 1.00 | 22.63 |
| ATOM | 2019 | CA  | LEU | A | 259 | 18.083 | 51.075 | 54.135 | 1.00 | 22.66 |
| ATOM | 2020 | C   | LEU | A | 259 | 18.266 | 51.673 | 55.530 | 1.00 | 25.16 |
| ATOM | 2021 | O   | LEU | A | 259 | 17.868 | 51.030 | 56.505 | 1.00 | 24.40 |
| ATOM | 2022 | CB  | LEU | A | 259 | 16.597 | 50.897 | 53.874 | 1.00 | 23.11 |
| ATOM | 2023 | CG  | LEU | A | 259 | 15.825 | 52.166 | 54.225 | 1.00 | 31.10 |
| ATOM | 2024 | CD1 | LEU | A | 259 | 16.317 | 53.352 | 53.395 | 1.00 | 30.78 |
| ATOM | 2025 | CD2 | LEU | A | 259 | 14.350 | 51.938 | 53.966 | 1.00 | 36.76 |
| ATOM | 2026 | N   | VAL | A | 260 | 18.858 | 52.889 | 55.615 | 1.00 | 18.62 |
| ATOM | 2027 | CA  | VAL | A | 260 | 19.068 | 53.580 | 56.888 | 1.00 | 19.24 |
| ATOM | 2028 | C   | VAL | A | 260 | 17.897 | 54.493 | 57.154 | 1.00 | 26.41 |
| ATOM | 2029 | O   | VAL | A | 260 | 17.739 | 55.527 | 56.516 | 1.00 | 28.56 |
| ATOM | 2030 | CB  | VAL | A | 260 | 20.372 | 54.347 | 56.891 | 1.00 | 22.59 |
| ATOM | 2031 | CG1 | VAL | A | 260 | 20.683 | 54.811 | 58.307 | 1.00 | 23.06 |
| ATOM | 2032 | CG2 | VAL | A | 260 | 21.488 | 53.433 | 56.439 | 1.00 | 21.80 |
| ATOM | 2033 | N   | LEU | A | 261 | 17.043 | 54.091 | 58.071 | 1.00 | 21.39 |
| ATOM | 2034 | CA  | LEU | A | 261 | 15.837 | 54.831 | 58.380 | 1.00 | 21.91 |
| ATOM | 2035 | C   | LEU | A | 261 | 16.041 | 56.017 | 59.301 | 1.00 | 26.50 |
| ATOM | 2036 | O   | LEU | A | 261 | 17.140 | 56.271 | 59.778 | 1.00 | 24.09 |
| ATOM | 2037 | CB  | LEU | A | 261 | 14.843 | 53.867 | 59.040 | 1.00 | 22.05 |
| ATOM | 2038 | CG  | LEU | A | 261 | 14.170 | 53.020 | 57.974 | 1.00 | 28.76 |
| ATOM | 2039 | CD1 | LEU | A | 261 | 14.886 | 51.690 | 57.819 | 1.00 | 30.80 |
| ATOM | 2040 | CD2 | LEU | A | 261 | 12.683 | 52.859 | 58.230 | 1.00 | 35.84 |
| ATOM | 2041 | N   | PRO | A | 262 | 14.946 | 56.724 | 59.565 | 1.00 | 27.39 |
| ATOM | 2042 | CA  | PRO | A | 262 | 14.989 | 57.844 | 60.482 | 1.00 | 24.71 |
| ATOM | 2043 | C   | PRO | A | 262 |        |        |        |      |       |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 2059 | CB  | SER | A | 264 | 11.281 | 57.498 | 65.183 | 1.00 | 23.65 |
| ATOM | 2060 | OG  | SER | A | 264 | 10.912 | 57.500 | 63.823 | 1.00 | 21.88 |
| ATOM | 2061 | N   | PHE | A | 265 | 13.175 | 54.762 | 64.054 | 1.00 | 17.44 |
| ATOM | 2062 | CA  | PHE | A | 265 | 12.995 | 53.336 | 63.775 | 1.00 | 16.88 |
| ATOM | 2063 | C   | PHE | A | 265 | 13.155 | 52.576 | 65.093 | 1.00 | 19.17 |
| ATOM | 2064 | O   | PHE | A | 265 | 14.149 | 52.730 | 65.785 | 1.00 | 19.42 |
| ATOM | 2065 | CB  | PHE | A | 265 | 13.962 | 52.852 | 62.696 | 1.00 | 18.72 |
| ATOM | 2066 | CG  | PHE | A | 265 | 13.632 | 51.450 | 62.311 | 1.00 | 20.49 |
| ATOM | 2067 | CD1 | PHE | A | 265 | 12.412 | 51.173 | 61.701 | 1.00 | 24.10 |
| ATOM | 2068 | CD2 | PHE | A | 265 | 14.527 | 50.413 | 62.564 | 1.00 | 23.76 |
| ATOM | 2069 | CE1 | PHE | A | 265 | 12.088 | 49.869 | 61.342 | 1.00 | 27.40 |
| ATOM | 2070 | CE2 | PHE | A | 265 | 14.210 | 49.100 | 62.218 | 1.00 | 28.74 |
| ATOM | 2071 | CZ  | PHE | A | 265 | 12.987 | 48.833 | 61.605 | 1.00 | 27.12 |
| ATOM | 2072 | N   | PRO | A | 266 | 12.158 | 51.803 | 65.451 | 1.00 | 18.02 |
| ATOM | 2073 | CA  | PRO | A | 266 | 12.110 | 51.080 | 66.718 | 1.00 | 18.74 |
| ATOM | 2074 | C   | PRO | A | 266 | 13.107 | 49.965 | 67.013 | 1.00 | 20.27 |
| ATOM | 2075 | O   | PRO | A | 266 | 13.293 | 49.635 | 68.170 | 1.00 | 15.77 |
| ATOM | 2076 | CB  | PRO | A | 266 | 10.696 | 50.520 | 66.822 | 1.00 | 20.13 |
| ATOM | 2077 | CG  | PRO | A | 266 | 10.127 | 50.546 | 65.416 | 1.00 | 23.78 |
| ATOM | 2078 | CD  | PRO | A | 266 | 10.967 | 51.531 | 64.615 | 1.00 | 19.11 |
| ATOM | 2079 | N   | TYR | A | 267 | 13.706 | 49.338 | 66.001 | 1.00 | 20.63 |
| ATOM | 2080 | CA  | TYR | A | 267 | 14.644 | 48.224 | 66.235 | 1.00 | 21.13 |
| ATOM | 2081 | C   | TYR | A | 267 | 16.031 | 48.497 | 65.651 | 1.00 | 22.74 |
| ATOM | 2082 | O   | TYR | A | 267 | 16.215 | 49.455 | 64.905 | 1.00 | 21.89 |
| ATOM | 2083 | CB  | TYR | A | 267 | 14.099 | 46.909 | 65.603 | 1.00 | 22.60 |
| ATOM | 2084 | CG  | TYR | A | 267 | 12.764 | 46.544 | 66.176 | 1.00 | 19.52 |
| ATOM | 2085 | CD1 | TYR | A | 267 | 12.726 | 45.858 | 67.389 | 1.00 | 19.63 |
| ATOM | 2086 | CD2 | TYR | A | 267 | 11.572 | 46.933 | 65.560 | 1.00 | 16.80 |
| ATOM | 2087 | CE1 | TYR | A | 267 | 11.507 | 45.541 | 67.987 | 1.00 | 21.00 |
| ATOM | 2088 | CE2 | TYR | A | 267 | 10.345 | 46.631 | 66.151 | 1.00 | 16.26 |
| ATOM | 2089 | CZ  | TYR | A | 267 | 10.322 | 45.924 | 67.360 | 1.00 | 21.79 |
| ATOM | 2090 | OH  | TYR | A | 267 | 9.143  | 45.605 | 67.993 | 1.00 | 24.21 |
| ATOM | 2091 | N   | GLY | A | 268 | 17.000 | 47.617 | 65.975 | 1.00 | 19.60 |
| ATOM | 2092 | CA  | GLY | A | 268 | 18.352 | 47.747 | 65.451 | 1.00 | 19.06 |
| ATOM | 2093 | C   | GLY | A | 268 | 18.283 | 47.578 | 63.946 | 1.00 | 21.42 |
| ATOM | 2094 | O   | GLY | A | 268 | 18.978 | 48.228 | 63.181 | 1.00 | 22.34 |
| ATOM | 2095 | N   | GLY | A | 269 | 17.396 | 46.686 | 63.510 | 1.00 | 20.52 |
| ATOM | 2096 | CA  | GLY | A | 269 | 17.230 | 46.448 | 62.098 | 1.00 | 22.99 |
| ATOM | 2097 | C   | GLY | A | 269 | 16.037 | 45.582 | 61.887 | 1.00 | 24.74 |
| ATOM | 2098 | O   | GLY | A | 269 | 15.439 | 45.139 | 62.853 | 1.00 | 21.33 |
| ATOM | 2099 | N   | MET | A | 270 | 15.707 | 45.343 | 60.640 | 1.00 | 17.60 |
| ATOM | 2100 | CA  | MET | A | 270 | 14.587 | 44.484 | 60.297 | 1.00 | 18.47 |
| ATOM | 2101 | C   | MET | A | 270 | 14.949 |        |        |      |       |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 2117 | CA  | ASN | A | 272 | 13.048 | 42.655 | 55.193 | 1.00 | 17.75 |
| ATOM | 2118 | C   | ASN | A | 272 | 13.790 | 42.114 | 54.010 | 1.00 | 17.01 |
| ATOM | 2119 | O   | ASN | A | 272 | 14.851 | 42.638 | 53.703 | 1.00 | 19.21 |
| ATOM | 2120 | CB  | ASN | A | 272 | 12.370 | 44.003 | 54.915 | 1.00 | 17.79 |
| ATOM | 2121 | CG  | ASN | A | 272 | 11.661 | 44.572 | 56.136 | 1.00 | 24.23 |
| ATOM | 2122 | OD1 | ASN | A | 272 | 11.907 | 45.714 | 56.563 | 1.00 | 37.07 |
| ATOM | 2123 | ND2 | ASN | A | 272 | 10.751 | 43.792 | 56.694 | 1.00 | 16.34 |
| ATOM | 2124 | N   | PRO | A | 273 | 13.261 | 41.060 | 53.393 | 1.00 | 16.33 |
| ATOM | 2125 | CA  | PRO | A | 273 | 13.943 | 40.451 | 52.265 | 1.00 | 17.34 |
| ATOM | 2126 | C   | PRO | A | 273 | 14.267 | 41.446 | 51.173 | 1.00 | 24.95 |
| ATOM | 2127 | O   | PRO | A | 273 | 13.431 | 42.244 | 50.757 | 1.00 | 26.24 |
| ATOM | 2128 | CB  | PRO | A | 273 | 13.064 | 39.333 | 51.737 | 1.00 | 19.31 |
| ATOM | 2129 | CG  | PRO | A | 273 | 11.797 | 39.328 | 52.569 | 1.00 | 22.96 |
| ATOM | 2130 | CD  | PRO | A | 273 | 11.925 | 40.459 | 53.588 | 1.00 | 16.97 |
| ATOM | 2131 | N   | CYS | A | 274 | 15.516 | 41.386 | 50.721 | 1.00 | 24.19 |
| ATOM | 2132 | CA  | CYS | A | 274 | 16.054 | 42.254 | 49.675 | 1.00 | 25.84 |
| ATOM | 2133 | C   | CYS | A | 274 | 16.278 | 43.666 | 50.140 | 1.00 | 27.71 |
| ATOM | 2134 | O   | CYS | A | 274 | 16.936 | 44.425 | 49.409 | 1.00 | 28.34 |
| ATOM | 2135 | CB  | CYS | A | 274 | 15.180 | 42.385 | 48.407 | 1.00 | 28.74 |
| ATOM | 2136 | SG  | CYS | A | 274 | 14.523 | 40.833 | 47.746 | 1.00 | 33.56 |
| ATOM | 2137 | N   | LEU | A | 275 | 15.724 | 44.015 | 51.305 | 1.00 | 21.22 |
| ATOM | 2138 | CA  | LEU | A | 275 | 15.832 | 45.374 | 51.803 | 1.00 | 20.67 |
| ATOM | 2139 | C   | LEU | A | 275 | 15.945 | 45.425 | 53.310 | 1.00 | 23.51 |
| ATOM | 2140 | O   | LEU | A | 275 | 14.982 | 45.644 | 54.033 | 1.00 | 18.39 |
| ATOM | 2141 | CB  | LEU | A | 275 | 14.631 | 46.228 | 51.307 | 1.00 | 20.52 |
| ATOM | 2142 | CG  | LEU | A | 275 | 14.710 | 47.769 | 51.456 | 1.00 | 24.37 |
| ATOM | 2143 | CD1 | LEU | A | 275 | 15.999 | 48.306 | 50.851 | 1.00 | 23.96 |
| ATOM | 2144 | CD2 | LEU | A | 275 | 13.543 | 48.414 | 50.707 | 1.00 | 29.41 |
| ATOM | 2145 | N   | THR | A | 276 | 17.155 | 45.224 | 53.790 | 1.00 | 26.98 |
| ATOM | 2146 | CA  | THR | A | 276 | 17.313 | 45.296 | 55.226 | 1.00 | 27.92 |
| ATOM | 2147 | C   | THR | A | 276 | 17.166 | 46.737 | 55.742 | 1.00 | 24.32 |
| ATOM | 2148 | O   | THR | A | 276 | 17.704 | 47.680 | 55.197 | 1.00 | 21.95 |
| ATOM | 2149 | CB  | THR | A | 276 | 18.635 | 44.667 | 55.732 | 1.00 | 28.74 |
| ATOM | 2150 | OG1 | THR | A | 276 | 18.526 | 43.261 | 55.810 | 1.00 | 29.92 |
| ATOM | 2151 | CG2 | THR | A | 276 | 18.941 | 45.171 | 57.132 | 1.00 | 23.98 |
| ATOM | 2152 | N   | PHE | A | 277 | 16.425 | 46.889 | 56.810 | 1.00 | 19.33 |
| ATOM | 2153 | CA  | PHE | A | 277 | 16.265 | 48.202 | 57.427 | 1.00 | 19.10 |
| ATOM | 2154 | C   | PHE | A | 277 | 17.203 | 48.239 | 58.632 | 1.00 | 26.76 |
| ATOM | 2155 | O   | PHE | A | 277 | 17.305 | 47.246 | 59.382 | 1.00 | 26.98 |
| ATOM | 2156 | CB  | PHE | A | 277 | 14.839 | 48.407 | 58.017 | 1.00 | 19.49 |
| ATOM | 2157 | CG  | PHE | A | 277 | 13.757 | 48.622 | 57.003 | 1.00 | 20.03 |
| ATOM | 2158 | CD1 | PHE | A | 277 | 13.966 | 48.271 | 55.668 | 1.00 | 24.06 |
| ATOM | 2159 | CD2 | PHE | A | 277 | 12.516 | 49.134 |        |      |       |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 2175 | OG1 | THR | A | 279 | 18.714 | 53.050 | 64.868 | 1.00 | 19.82 |
| ATOM | 2176 | CG2 | THR | A | 279 | 19.964 | 51.004 | 64.542 | 1.00 | 16.49 |
| ATOM | 2177 | N   | PRO | A | 280 | 19.702 | 54.306 | 62.335 | 1.00 | 24.27 |
| ATOM | 2178 | CA  | PRO | A | 280 | 20.833 | 55.201 | 62.087 | 1.00 | 22.03 |
| ATOM | 2179 | C   | PRO | A | 280 | 21.748 | 55.222 | 63.312 | 1.00 | 23.36 |
| ATOM | 2180 | O   | PRO | A | 280 | 22.871 | 55.758 | 63.265 | 1.00 | 22.67 |
| ATOM | 2181 | CB  | PRO | A | 280 | 20.272 | 56.603 | 61.813 | 1.00 | 22.22 |
| ATOM | 2182 | CG  | PRO | A | 280 | 18.766 | 56.520 | 62.043 | 1.00 | 27.67 |
| ATOM | 2183 | CD  | PRO | A | 280 | 18.397 | 55.053 | 62.250 | 1.00 | 23.53 |
| ATOM | 2184 | N   | THR | A | 281 | 21.266 | 54.616 | 64.405 | 1.00 | 17.56 |
| ATOM | 2185 | CA  | THR | A | 281 | 22.082 | 54.545 | 65.602 | 1.00 | 17.27 |
| ATOM | 2186 | C   | THR | A | 281 | 23.287 | 53.665 | 65.362 | 1.00 | 21.93 |
| ATOM | 2187 | O   | THR | A | 281 | 24.183 | 53.597 | 66.199 | 1.00 | 20.04 |
| ATOM | 2188 | CB  | THR | A | 281 | 21.373 | 54.112 | 66.902 | 1.00 | 17.56 |
| ATOM | 2189 | OG1 | THR | A | 281 | 20.857 | 52.799 | 66.785 | 1.00 | 21.89 |
| ATOM | 2190 | CG2 | THR | A | 281 | 20.283 | 55.142 | 67.261 | 1.00 | 21.96 |
| ATOM | 2191 | N   | LEU | A | 282 | 23.312 | 52.977 | 64.232 | 1.00 | 17.97 |
| ATOM | 2192 | CA  | LEU | A | 282 | 24.487 | 52.135 | 63.947 | 1.00 | 17.90 |
| ATOM | 2193 | C   | LEU | A | 282 | 25.696 | 52.965 | 63.437 | 1.00 | 22.56 |
| ATOM | 2194 | O   | LEU | A | 282 | 26.821 | 52.478 | 63.352 | 1.00 | 22.13 |
| ATOM | 2195 | CB  | LEU | A | 282 | 24.206 | 51.077 | 62.864 | 1.00 | 15.83 |
| ATOM | 2196 | CG  | LEU | A | 282 | 23.051 | 50.117 | 63.132 | 1.00 | 21.56 |
| ATOM | 2197 | CD1 | LEU | A | 282 | 23.068 | 49.007 | 62.079 | 1.00 | 20.06 |
| ATOM | 2198 | CD2 | LEU | A | 282 | 23.201 | 49.502 | 64.507 | 1.00 | 17.47 |
| ATOM | 2199 | N   | LEU | A | 283 | 25.452 | 54.219 | 63.053 | 1.00 | 20.88 |
| ATOM | 2200 | CA  | LEU | A | 283 | 26.501 | 55.049 | 62.479 | 1.00 | 21.60 |
| ATOM | 2201 | C   | LEU | A | 283 | 27.522 | 55.554 | 63.463 | 1.00 | 29.62 |
| ATOM | 2202 | O   | LEU | A | 283 | 27.624 | 56.755 | 63.633 | 1.00 | 31.93 |
| ATOM | 2203 | CB  | LEU | A | 283 | 25.895 | 56.225 | 61.682 | 1.00 | 21.41 |
| ATOM | 2204 | CG  | LEU | A | 283 | 24.839 | 55.780 | 60.662 | 1.00 | 24.34 |
| ATOM | 2205 | CD1 | LEU | A | 283 | 24.230 | 57.001 | 59.956 | 1.00 | 23.79 |
| ATOM | 2206 | CD2 | LEU | A | 283 | 25.480 | 54.835 | 59.639 | 1.00 | 26.70 |
| ATOM | 2207 | N   | ALA | A | 284 | 28.271 | 54.652 | 64.118 | 1.00 | 26.89 |
| ATOM | 2208 | CA  | ALA | A | 284 | 29.257 | 55.077 | 65.103 | 1.00 | 24.30 |
| ATOM | 2209 | C   | ALA | A | 284 | 30.467 | 55.770 | 64.477 | 1.00 | 29.39 |
| ATOM | 2210 | O   | ALA | A | 284 | 31.203 | 56.476 | 65.155 | 1.00 | 31.04 |
| ATOM | 2211 | CB  | ALA | A | 284 | 29.694 | 53.941 | 66.015 | 1.00 | 24.10 |
| ATOM | 2212 | N   | GLY | A | 285 | 30.694 | 55.561 | 63.180 | 1.00 | 22.20 |
| ATOM | 2213 | CA  | GLY | A | 285 | 31.822 | 56.190 | 62.534 | 1.00 | 21.17 |
| ATOM | 2214 | C   | GLY | A | 285 | 33.061 | 55.295 | 62.386 | 1.00 | 31.73 |
| ATOM | 2215 | O   | GLY | A | 285 | 34.013 | 55.659 | 61.696 | 1.00 | 32.59 |
| ATOM | 2216 | N   | ASP | A | 286 | 33.063 | 54.105 | 63.020 | 1.00 | 28.41 |
| ATOM | 2217 | CA  | ASP | A | 286 | 34.184 | 53.180 | 62.939 | 1.00 | 21.98 |
| ATOM | 2218 | C   | ASP | A | 286 | 33.757 | 51.763 | 62.583 | 1.00 | 25.41 |
| ATOM | 2219 | O   | ASP | A | 286 | 34.532 | 50.834 | 62.765 | 1.00 | 24.81 |
| ATOM | 2220 | CB  | ASP | A | 286 | 34.906 | 53.146 | 64.268 | 1.00 | 22.94 |
| ATOM | 2221 | CG  | ASP | A | 286 | 33.959 | 52.719 | 65.334 | 1.00 | 33.17 |
| ATOM | 2222 | OD1 | ASP | A | 286 | 32.821 | 52.362 | 65.097 | 1.00 | 32.35 |
| ATOM | 2223 | OD2 | ASP | A | 286 | 34.492 | 52.744 | 66.523 | 1.00 | 37.83 |
| ATOM | 2224 | N   | LYS | A | 287 | 32.512 | 51.605 | 62.122 | 1.00 | 23.26 |
| ATOM | 2225 | CA  | LYS | A | 287 | 31.988 | 50.297 | 61.719 | 1.00 | 23.59 |
| ATOM | 2226 | C   | LYS | A | 287 | 31.865 | 49.336 | 62.888 | 1.00 | 24.51 |
| ATOM | 2227 | O   | LYS | A | 287 | 31.681 | 48.136 | 62.711 | 1.00 | 23.45 |
| ATOM | 2228 | CB  | LYS | A | 287 | 32.918 | 49.636 | 60.694 | 1.00 | 24.58 |
| ATOM | 2229 | CG  | LYS | A | 287 | 33.510 | 50.531 | 59.618 | 1.00 | 29.73 |
| ATOM | 2230 | CD  | LYS | A | 287 | 34.297 | 49.706 | 58.598 | 1.00 | 34.17 |
| ATOM | 2231 | CE  | LYS | A | 287 | 35.044 | 50.517 | 57.572 | 1.00 | 33.69 |
| ATOM | 2232 | NZ  | LYS | A | 287 | 34.164 | 51.281 | 56.664 | 1.00 | 36.75 |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 2233 | N   | SER | A | 288 | 31.972 | 49.866 | 64.091 | 1.00 | 23.33 |
| ATOM | 2234 | CA  | SER | A | 288 | 31.941 | 49.045 | 65.285 | 1.00 | 20.21 |
| ATOM | 2235 | C   | SER | A | 288 | 30.649 | 48.286 | 65.585 | 1.00 | 26.52 |
| ATOM | 2236 | O   | SER | A | 288 | 30.671 | 47.247 | 66.272 | 1.00 | 24.43 |
| ATOM | 2237 | CB  | SER | A | 288 | 32.482 | 49.805 | 66.483 | 1.00 | 18.45 |
| ATOM | 2238 | OG  | SER | A | 288 | 31.558 | 50.812 | 66.797 | 1.00 | 27.86 |
| ATOM | 2239 | N   | LEU | A | 289 | 29.519 | 48.791 | 65.088 | 1.00 | 23.04 |
| ATOM | 2240 | CA  | LEU | A | 289 | 28.247 | 48.129 | 65.338 | 1.00 | 21.77 |
| ATOM | 2241 | C   | LEU | A | 289 | 27.781 | 47.281 | 64.165 | 1.00 | 24.87 |
| ATOM | 2242 | O   | LEU | A | 289 | 26.595 | 46.999 | 63.993 | 1.00 | 23.49 |
| ATOM | 2243 | CB  | LEU | A | 289 | 27.169 | 49.134 | 65.733 | 1.00 | 21.62 |
| ATOM | 2244 | CG  | LEU | A | 289 | 27.655 | 50.085 | 66.804 | 1.00 | 24.32 |
| ATOM | 2245 | CD1 | LEU | A | 289 | 26.587 | 51.127 | 67.041 | 1.00 | 22.74 |
| ATOM | 2246 | CD2 | LEU | A | 289 | 27.900 | 49.299 | 68.090 | 1.00 | 23.03 |
| ATOM | 2247 | N   | SER | A | 290 | 28.735 | 46.867 | 63.358 | 1.00 | 22.75 |
| ATOM | 2248 | CA  | SER | A | 290 | 28.418 | 46.074 | 62.203 | 1.00 | 22.55 |
| ATOM | 2249 | C   | SER | A | 290 | 27.840 | 44.715 | 62.577 | 1.00 | 26.48 |
| ATOM | 2250 | O   | SER | A | 290 | 27.240 | 44.047 | 61.729 | 1.00 | 25.78 |
| ATOM | 2251 | CB  | SER | A | 290 | 29.619 | 45.960 | 61.293 | 1.00 | 23.90 |
| ATOM | 2252 | OG  | SER | A | 290 | 30.468 | 44.969 | 61.839 | 1.00 | 38.79 |
| ATOM | 2253 | N   | ASN | A | 291 | 27.990 | 44.285 | 63.845 | 1.00 | 19.29 |
| ATOM | 2254 | CA  | ASN | A | 291 | 27.407 | 42.997 | 64.158 | 1.00 | 19.36 |
| ATOM | 2255 | C   | ASN | A | 291 | 25.942 | 43.006 | 63.785 | 1.00 | 25.06 |
| ATOM | 2256 | O   | ASN | A | 291 | 25.372 | 41.981 | 63.398 | 1.00 | 23.17 |
| ATOM | 2257 | CB  | ASN | A | 291 | 27.578 | 42.553 | 65.608 | 1.00 | 16.45 |
| ATOM | 2258 | CG  | ASN | A | 291 | 26.714 | 43.390 | 66.488 | 1.00 | 21.86 |
| ATOM | 2259 | OD1 | ASN | A | 291 | 26.958 | 44.565 | 66.626 | 1.00 | 24.59 |
| ATOM | 2260 | ND2 | ASN | A | 291 | 25.646 | 42.794 | 67.012 | 1.00 | 27.34 |
| ATOM | 2261 | N   | VAL | A | 292 | 25.323 | 44.184 | 63.885 | 1.00 | 21.23 |
| ATOM | 2262 | CA  | VAL | A | 292 | 23.903 | 44.282 | 63.564 | 1.00 | 17.12 |
| ATOM | 2263 | C   | VAL | A | 292 | 23.651 | 43.926 | 62.113 | 1.00 | 22.88 |
| ATOM | 2264 | O   | VAL | A | 292 | 22.639 | 43.320 | 61.751 | 1.00 | 24.23 |
| ATOM | 2265 | CB  | VAL | A | 292 | 23.306 | 45.616 | 63.957 | 1.00 | 19.41 |
| ATOM | 2266 | CG1 | VAL | A | 292 | 21.861 | 45.660 | 63.492 | 1.00 | 19.16 |
| ATOM | 2267 | CG2 | VAL | A | 292 | 23.353 | 45.733 | 65.468 | 1.00 | 17.97 |
| ATOM | 2268 | N   | ILE | A | 293 | 24.599 | 44.292 | 61.269 | 1.00 | 20.25 |
| ATOM | 2269 | CA  | ILE | A | 293 | 24.465 | 43.971 | 59.867 | 1.00 | 20.49 |
| ATOM | 2270 | C   | ILE | A | 293 | 24.578 | 42.426 | 59.655 | 1.00 | 24.54 |
| ATOM | 2271 | O   | ILE | A | 293 | 23.801 | 41.780 | 58.903 | 1.00 | 22.05 |
| ATOM | 2272 | CB  | ILE | A | 293 | 25.488 | 44.762 | 59.038 | 1.00 | 24.97 |
| ATOM | 2273 | CG1 | ILE | A | 293 | 25.299 | 46.274 | 59.158 | 1.00 | 22.05 |
| ATOM | 2274 | CG2 | ILE | A | 293 | 25.301 | 44.415 | 57.576 | 1.00 | 29.49 |
| ATOM | 2275 | CD1 | ILE | A | 293 | 23.950 | 46.712 |        |      |       |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 2291 | N   | GLU | A | 296 | 21.252 | 40.868 | 60.547 | 1.00 | 14.96 |
| ATOM | 2292 | CA  | GLU | A | 296 | 20.222 | 40.959 | 59.515 | 1.00 | 17.03 |
| ATOM | 2293 | C   | GLU | A | 296 | 20.529 | 40.090 | 58.323 | 1.00 | 20.56 |
| ATOM | 2294 | O   | GLU | A | 296 | 19.624 | 39.500 | 57.744 | 1.00 | 22.06 |
| ATOM | 2295 | CB  | GLU | A | 296 | 19.900 | 42.402 | 59.052 | 1.00 | 18.78 |
| ATOM | 2296 | CG  | GLU | A | 296 | 19.607 | 43.415 | 60.181 | 1.00 | 17.76 |
| ATOM | 2297 | CD  | GLU | A | 296 | 18.765 | 42.905 | 61.324 | 1.00 | 26.07 |
| ATOM | 2298 | OE1 | GLU | A | 296 | 18.010 | 41.975 | 61.243 | 1.00 | 24.13 |
| ATOM | 2299 | OE2 | GLU | A | 296 | 18.874 | 43.640 | 62.413 | 1.00 | 42.10 |
| ATOM | 2300 | N   | ILE | A | 297 | 21.799 | 40.001 | 57.957 | 1.00 | 16.85 |
| ATOM | 2301 | CA  | ILE | A | 297 | 22.176 | 39.161 | 56.846 | 1.00 | 15.16 |
| ATOM | 2302 | C   | ILE | A | 297 | 21.825 | 37.709 | 57.169 | 1.00 | 22.46 |
| ATOM | 2303 | O   | ILE | A | 297 | 21.310 | 36.919 | 56.339 | 1.00 | 18.88 |
| ATOM | 2304 | CB  | ILE | A | 297 | 23.676 | 39.273 | 56.680 | 1.00 | 17.58 |
| ATOM | 2305 | CG1 | ILE | A | 297 | 24.051 | 40.492 | 55.842 | 1.00 | 17.94 |
| ATOM | 2306 | CG2 | ILE | A | 297 | 24.194 | 38.001 | 56.047 | 1.00 | 16.21 |
| ATOM | 2307 | CD1 | ILE | A | 297 | 25.558 | 40.688 | 55.777 | 1.00 | 16.70 |
| ATOM | 2308 | N   | SER | A | 298 | 22.126 | 37.334 | 58.419 | 1.00 | 16.91 |
| ATOM | 2309 | CA  | SER | A | 298 | 21.857 | 35.952 | 58.836 | 1.00 | 16.01 |
| ATOM | 2310 | C   | SER | A | 298 | 20.402 | 35.530 | 58.690 | 1.00 | 18.70 |
| ATOM | 2311 | O   | SER | A | 298 | 20.129 | 34.360 | 58.355 | 1.00 | 18.32 |
| ATOM | 2312 | CB  | SER | A | 298 | 22.365 | 35.647 | 60.222 | 1.00 | 18.04 |
| ATOM | 2313 | OG  | SER | A | 298 | 23.759 | 35.843 | 60.212 | 1.00 | 25.50 |
| ATOM | 2314 | N   | HIS | A | 299 | 19.496 | 36.484 | 58.951 | 1.00 | 16.60 |
| ATOM | 2315 | CA  | HIS | A | 299 | 18.064 | 36.277 | 58.849 | 1.00 | 16.43 |
| ATOM | 2316 | C   | HIS | A | 299 | 17.660 | 35.796 | 57.454 | 1.00 | 20.34 |
| ATOM | 2317 | O   | HIS | A | 299 | 16.580 | 35.206 | 57.285 | 1.00 | 19.75 |
| ATOM | 2318 | CB  | HIS | A | 299 | 17.252 | 37.538 | 59.241 | 1.00 | 15.73 |
| ATOM | 2319 | CG  | HIS | A | 299 | 16.941 | 37.599 | 60.709 | 1.00 | 18.61 |
| ATOM | 2320 | ND1 | HIS | A | 299 | 16.410 | 36.500 | 61.393 | 1.00 | 18.57 |
| ATOM | 2321 | CD2 | HIS | A | 299 | 17.108 | 38.612 | 61.617 | 1.00 | 19.47 |
| ATOM | 2322 | CE1 | HIS | A | 299 | 16.265 | 36.863 | 62.660 | 1.00 | 16.96 |
| ATOM | 2323 | NE2 | HIS | A | 299 | 16.665 | 38.109 | 62.818 | 1.00 | 18.81 |
| ATOM | 2324 | N   | SER | A | 300 | 18.516 | 36.060 | 56.460 | 1.00 | 16.40 |
| ATOM | 2325 | CA  | SER | A | 300 | 18.231 | 35.641 | 55.084 | 1.00 | 19.81 |
| ATOM | 2326 | C   | SER | A | 300 | 18.105 | 34.120 | 54.951 | 1.00 | 25.93 |
| ATOM | 2327 | O   | SER | A | 300 | 17.626 | 33.597 | 53.936 | 1.00 | 23.71 |
| ATOM | 2328 | CB  | SER | A | 300 | 19.240 | 36.184 | 54.064 | 1.00 | 27.33 |
| ATOM | 2329 | OG  | SER | A | 300 | 19.323 | 37.591 | 54.135 | 1.00 | 26.20 |
| ATOM | 2330 | N   | TRP | A | 301 | 18.564 | 33.415 | 55.994 | 1.00 | 23.64 |
| ATOM | 2331 | CA  | TRP | A | 301 | 18.480 | 31.980 | 56.072 | 1.00 | 23.37 |
| ATOM | 2332 | C   | TRP | A | 301 | 17.579 | 31.598 | 57.249 | 1.00 | 27.41 |
| ATOM | 2333 | O   | TRP | A | 301 | 16.503 | 31.014 | 57.072 | 1.00 | 26.23 |
| ATOM | 2334 | CB  | TRP | A | 301 | 19.866 | 31.334 | 56.222 | 1.00 | 22.22 |
| ATOM | 2335 | CG  | TRP | A | 301 | 20.722 | 31.499 | 55.000 | 1.00 | 25.34 |
| ATOM | 2336 | CD1 | TRP | A | 301 | 20.897 | 30.577 | 53.999 | 1.00 | 28.73 |
| ATOM | 2337 | CD2 | TRP | A | 301 | 21.534 | 32.613 | 54.641 | 1.00 | 23.93 |
| ATOM | 2338 | NE1 | TRP | A | 301 | 21.743 | 31.051 | 53.032 | 1.00 | 25.58 |
| ATOM | 2339 | CE2 | TRP | A | 301 | 22.156 | 32.295 | 53.396 | 1.00 | 24.57 |
| ATOM | 2340 | CE3 | TRP | A | 301 | 21.778 | 33.847 | 55.244 | 1.00 | 24.02 |
| ATOM | 2341 | CZ2 | TRP | A | 301 | 23.010 | 33.177 | 52.743 | 1.00 | 23.11 |
| ATOM | 2342 | CZ3 | TRP | A | 301 | 22.609 | 34.727 | 54.586 | 1.00 | 25.68 |
| ATOM | 2343 | CH2 | TRP | A | 301 | 23.232 | 34.385 | 53.368 | 1.00 | 26.71 |
| ATOM | 2344 | N   | THR | A | 302 | 18.030 | 31.964 | 58.469 | 1.00 | 23.13 |
| ATOM | 2345 | CA  | THR | A | 302 | 17.299 | 31.646 | 59.698 | 1.00 | 20.44 |
| ATOM | 2346 | C   | THR | A | 302 | 16.314 | 32.722 | 60.004 | 1.00 | 23.69 |
| ATOM | 2347 | O   | THR | A | 302 | 16.673 | 33.739 | 60.555 | 1.00 | 23.66 |
| ATOM | 2348 | CB  | THR | A | 302 | 18.238 | 31.327 | 60.891 | 1.00 | 27.33 |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 2349 | OG1 | THR | A | 302 | 19.190 | 32.355 | 61.052 | 1.00 | 21.35 |
| ATOM | 2350 | CG2 | THR | A | 302 | 18.973 | 30.007 | 60.646 | 1.00 | 22.24 |
| ATOM | 2351 | N   | GLY | A | 303 | 15.070 | 32.492 | 59.620 | 1.00 | 19.58 |
| ATOM | 2352 | CA  | GLY | A | 303 | 14.004 | 33.460 | 59.800 | 1.00 | 16.06 |
| ATOM | 2353 | C   | GLY | A | 303 | 13.286 | 33.658 | 58.468 | 1.00 | 19.82 |
| ATOM | 2354 | O   | GLY | A | 303 | 12.092 | 33.388 | 58.365 | 1.00 | 19.83 |
| ATOM | 2355 | N   | ASN | A | 304 | 14.017 | 34.119 | 57.444 | 1.00 | 16.86 |
| ATOM | 2356 | CA  | ASN | A | 304 | 13.399 | 34.321 | 56.143 | 1.00 | 16.61 |
| ATOM | 2357 | C   | ASN | A | 304 | 13.238 | 33.035 | 55.347 | 1.00 | 23.54 |
| ATOM | 2358 | O   | ASN | A | 304 | 12.223 | 32.894 | 54.652 | 1.00 | 21.34 |
| ATOM | 2359 | CB  | ASN | A | 304 | 14.043 | 35.434 | 55.308 | 1.00 | 14.57 |
| ATOM | 2360 | CG  | ASN | A | 304 | 14.108 | 36.721 | 56.098 | 1.00 | 25.16 |
| ATOM | 2361 | OD1 | ASN | A | 304 | 13.623 | 36.756 | 57.255 | 1.00 | 20.16 |
| ATOM | 2362 | ND2 | ASN | A | 304 | 14.648 | 37.782 | 55.467 | 1.00 | 21.15 |
| ATOM | 2363 | N   | LEU | A | 305 | 14.216 | 32.090 | 55.431 | 1.00 | 19.86 |
| ATOM | 2364 | CA  | LEU | A | 305 | 14.049 | 30.819 | 54.669 | 1.00 | 20.27 |
| ATOM | 2365 | C   | LEU | A | 305 | 13.273 | 29.810 | 55.496 | 1.00 | 24.31 |
| ATOM | 2366 | O   | LEU | A | 305 | 12.282 | 29.233 | 55.044 | 1.00 | 21.45 |
| ATOM | 2367 | CB  | LEU | A | 305 | 15.352 | 30.177 | 54.176 | 1.00 | 21.11 |
| ATOM | 2368 | CG  | LEU | A | 305 | 15.786 | 30.655 | 52.809 | 1.00 | 25.81 |
| ATOM | 2369 | CD1 | LEU | A | 305 | 17.105 | 29.986 | 52.465 | 1.00 | 23.53 |
| ATOM | 2370 | CD2 | LEU | A | 305 | 14.713 | 30.354 | 51.766 | 1.00 | 25.44 |
| ATOM | 2371 | N   | VAL | A | 306 | 13.766 | 29.600 | 56.715 | 1.00 | 19.66 |
| ATOM | 2372 | CA  | VAL | A | 306 | 13.116 | 28.715 | 57.667 | 1.00 | 19.73 |
| ATOM | 2373 | C   | VAL | A | 306 | 12.540 | 29.643 | 58.716 | 1.00 | 23.65 |
| ATOM | 2374 | O   | VAL | A | 306 | 13.250 | 30.390 | 59.389 | 1.00 | 21.08 |
| ATOM | 2375 | CB  | VAL | A | 306 | 13.955 | 27.552 | 58.203 | 1.00 | 24.56 |
| ATOM | 2376 | CG1 | VAL | A | 306 | 15.439 | 27.775 | 58.065 | 1.00 | 25.21 |
| ATOM | 2377 | CG2 | VAL | A | 306 | 13.546 | 27.071 | 59.593 | 1.00 | 23.12 |
| ATOM | 2378 | N   | THR | A | 307 | 11.227 | 29.653 | 58.786 | 1.00 | 22.38 |
| ATOM | 2379 | CA  | THR | A | 307 | 10.491 | 30.569 | 59.652 | 1.00 | 18.69 |
| ATOM | 2380 | C   | THR | A | 307 | 9.776  | 29.908 | 60.803 | 1.00 | 19.89 |
| ATOM | 2381 | O   | THR | A | 307 | 9.265  | 28.797 | 60.676 | 1.00 | 18.85 |
| ATOM | 2382 | CB  | THR | A | 307 | 9.440  | 31.242 | 58.731 | 1.00 | 16.78 |
| ATOM | 2383 | OG1 | THR | A | 307 | 10.099 | 31.705 | 57.575 | 1.00 | 21.78 |
| ATOM | 2384 | CG2 | THR | A | 307 | 8.767  | 32.425 | 59.408 | 1.00 | 14.70 |
| ATOM | 2385 | N   | ASN | A | 308 | 9.719  | 30.607 | 61.934 | 1.00 | 15.56 |
| ATOM | 2386 | CA  | ASN | A | 308 | 9.007  | 30.068 | 63.069 | 1.00 | 14.26 |
| ATOM | 2387 | C   | ASN | A | 308 | 7.534  | 29.908 | 62.638 | 1.00 | 17.86 |
| ATOM | 2388 | O   | ASN | A | 308 | 6.972  | 30.743 | 61.911 | 1.00 | 19.31 |
| ATOM | 2389 | CB  | ASN | A | 308 | 9.214  | 30.967 | 64.327 | 1.00 | 14.46 |
| ATOM | 2390 | CG  | ASN | A | 308 | 9.026  | 32.476 | 64.197 | 1.00 | 23.32 |
| ATOM | 2391 | OD1 | ASN | A | 308 | 9.548  | 33.245 | 65     |      |       |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 2407 | OG1 | THR | A | 310 | 3.625  | 29.509 | 67.381 | 1.00 | 20.97 |
| ATOM | 2408 | CG2 | THR | A | 310 | 2.148  | 29.053 | 65.492 | 1.00 | 22.03 |
| ATOM | 2409 | N   | TRP | A | 311 | 4.640  | 32.649 | 66.669 | 1.00 | 16.83 |
| ATOM | 2410 | CA  | TRP | A | 311 | 5.531  | 33.473 | 67.477 | 1.00 | 13.87 |
| ATOM | 2411 | C   | TRP | A | 311 | 5.957  | 32.812 | 68.766 | 1.00 | 14.72 |
| ATOM | 2412 | O   | TRP | A | 311 | 6.891  | 33.247 | 69.422 | 1.00 | 15.63 |
| ATOM | 2413 | CB  | TRP | A | 311 | 4.904  | 34.837 | 67.698 | 1.00 | 12.94 |
| ATOM | 2414 | CG  | TRP | A | 311 | 4.716  | 35.521 | 66.410 | 1.00 | 14.94 |
| ATOM | 2415 | CD1 | TRP | A | 311 | 3.536  | 35.917 | 65.896 | 1.00 | 17.72 |
| ATOM | 2416 | CD2 | TRP | A | 311 | 5.744  | 35.880 | 65.459 | 1.00 | 17.04 |
| ATOM | 2417 | NE1 | TRP | A | 311 | 3.739  | 36.531 | 64.685 | 1.00 | 19.20 |
| ATOM | 2418 | CE2 | TRP | A | 311 | 5.092  | 36.531 | 64.384 | 1.00 | 21.28 |
| ATOM | 2419 | CE3 | TRP | A | 311 | 7.135  | 35.723 | 65.408 | 1.00 | 18.68 |
| ATOM | 2420 | CZ2 | TRP | A | 311 | 5.792  | 37.000 | 63.260 | 1.00 | 18.99 |
| ATOM | 2421 | CZ3 | TRP | A | 311 | 7.813  | 36.210 | 64.309 | 1.00 | 19.24 |
| ATOM | 2422 | CH2 | TRP | A | 311 | 7.151  | 36.841 | 63.247 | 1.00 | 18.58 |
| ATOM | 2423 | N   | ASP | A | 312 | 5.285  | 31.739 | 69.136 | 1.00 | 14.32 |
| ATOM | 2424 | CA  | ASP | A | 312 | 5.677  | 31.022 | 70.355 | 1.00 | 16.52 |
| ATOM | 2425 | C   | ASP | A | 312 | 7.057  | 30.348 | 70.182 | 1.00 | 20.97 |
| ATOM | 2426 | O   | ASP | A | 312 | 7.728  | 30.022 | 71.141 | 1.00 | 16.88 |
| ATOM | 2427 | CB  | ASP | A | 312 | 4.644  | 29.947 | 70.744 | 1.00 | 18.67 |
| ATOM | 2428 | CG  | ASP | A | 312 | 3.331  | 30.475 | 71.277 | 1.00 | 24.42 |
| ATOM | 2429 | OD1 | ASP | A | 312 | 3.179  | 31.578 | 71.761 | 1.00 | 26.54 |
| ATOM | 2430 | OD2 | ASP | A | 312 | 2.390  | 29.579 | 71.220 | 1.00 | 32.52 |
| ATOM | 2431 | N   | HIS | A | 313 | 7.447  | 30.132 | 68.919 | 1.00 | 16.31 |
| ATOM | 2432 | CA  | HIS | A | 313 | 8.688  | 29.503 | 68.532 | 1.00 | 13.00 |
| ATOM | 2433 | C   | HIS | A | 313 | 9.717  | 30.498 | 68.007 | 1.00 | 17.41 |
| ATOM | 2434 | O   | HIS | A | 313 | 10.670 | 30.160 | 67.348 | 1.00 | 19.76 |
| ATOM | 2435 | CB  | HIS | A | 313 | 8.337  | 28.435 | 67.454 | 1.00 | 14.66 |
| ATOM | 2436 | CG  | HIS | A | 313 | 7.461  | 27.395 | 68.061 | 1.00 | 17.94 |
| ATOM | 2437 | ND1 | HIS | A | 313 | 7.980  | 26.389 | 68.863 | 1.00 | 19.58 |
| ATOM | 2438 | CD2 | HIS | A | 313 | 6.110  | 27.278 | 68.054 | 1.00 | 18.14 |
| ATOM | 2439 | CE1 | HIS | A | 313 | 6.946  | 25.663 | 69.305 | 1.00 | 18.62 |
| ATOM | 2440 | NE2 | HIS | A | 313 | 5.811  | 26.178 | 68.828 | 1.00 | 18.86 |
| ATOM | 2441 | N   | PHE | A | 314 | 9.532  | 31.752 | 68.337 | 1.00 | 17.04 |
| ATOM | 2442 | CA  | PHE | A | 314 | 10.391 | 32.850 | 67.928 | 1.00 | 14.60 |
| ATOM | 2443 | C   | PHE | A | 314 | 11.861 | 32.591 | 68.188 | 1.00 | 14.03 |
| ATOM | 2444 | O   | PHE | A | 314 | 12.756 | 33.089 | 67.509 | 1.00 | 15.80 |
| ATOM | 2445 | CB  | PHE | A | 314 | 9.943  | 34.129 | 68.656 | 1.00 | 15.67 |
| ATOM | 2446 | CG  | PHE | A | 314 | 10.618 | 35.416 | 68.185 | 1.00 | 17.93 |
| ATOM | 2447 | CD1 | PHE | A | 314 | 10.734 | 35.717 | 66.826 | 1.00 | 17.79 |
| ATOM | 2448 | CD2 | PHE | A | 314 | 11.111 | 36.344 | 69.116 | 1.00 | 17.04 |
| ATOM | 2449 | CE1 | PHE | A | 314 | 11.336 | 36.910 | 66.418 | 1.00 | 17.88 |
| ATOM | 2450 | CE2 | PHE | A | 314 | 11.721 | 37.538 | 68.720 | 1.00 | 17.77 |
| ATOM | 2451 | CZ  | PHE | A | 314 | 11.824 | 37.822 | 67.358 | 1.00 | 15.05 |
| ATOM | 2452 | N   | TRP | A | 315 | 12.145 | 31.812 | 69.177 | 1.00 | 14.30 |
| ATOM | 2453 | CA  | TRP | A | 315 | 13.551 | 31.581 | 69.445 | 1.00 | 13.26 |
| ATOM | 2454 | C   | TRP | A | 315 | 14.219 | 30.940 | 68.255 | 1.00 | 17.26 |
| ATOM | 2455 | O   | TRP | A | 315 | 15.391 | 31.153 | 68.003 | 1.00 | 16.79 |
| ATOM | 2456 | CB  | TRP | A | 315 | 13.805 | 30.797 | 70.763 | 1.00 | 13.36 |
| ATOM | 2457 | CG  | TRP | A | 315 | 13.608 | 29.330 | 70.603 | 1.00 | 15.85 |
| ATOM | 2458 | CD1 | TRP | A | 315 | 12.425 | 28.660 | 70.644 | 1.00 | 19.09 |
| ATOM | 2459 | CD2 | TRP | A | 315 | 14.612 | 28.351 | 70.278 | 1.00 | 16.53 |
| ATOM | 2460 | NE1 | TRP | A | 315 | 12.631 | 27.325 | 70.422 | 1.00 | 18.83 |
| ATOM | 2461 | CE2 | TRP | A | 315 | 13.968 | 27.108 | 70.161 | 1.00 | 20.33 |
| ATOM | 2462 | CE3 | TRP | A | 315 | 15.981 | 28.411 | 70.051 | 1.00 | 16.71 |
| ATOM | 2463 | CZ2 | TRP | A | 315 | 14.671 | 25.924 | 69.865 | 1.00 | 18.62 |
| ATOM | 2464 | CZ3 | TRP | A | 315 | 16.664 | 27.238 | 69.777 | 1.00 | 17.58 |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 2465 | CH2 | TRP | A | 315 | 16.027 | 26.004 | 69.680 | 1.00 | 16.98 |
| ATOM | 2466 | N   | LEU | A | 316 | 13.490 | 30.115 | 67.508 | 1.00 | 16.82 |
| ATOM | 2467 | CA  | LEU | A | 316 | 14.126 | 29.478 | 66.367 | 1.00 | 16.28 |
| ATOM | 2468 | C   | LEU | A | 316 | 14.705 | 30.543 | 65.434 | 1.00 | 19.17 |
| ATOM | 2469 | O   | LEU | A | 316 | 15.820 | 30.419 | 64.920 | 1.00 | 20.97 |
| ATOM | 2470 | CB  | LEU | A | 316 | 13.125 | 28.610 | 65.569 | 1.00 | 15.83 |
| ATOM | 2471 | CG  | LEU | A | 316 | 12.628 | 27.362 | 66.276 | 1.00 | 18.57 |
| ATOM | 2472 | CD1 | LEU | A | 316 | 11.532 | 26.714 | 65.422 | 1.00 | 16.74 |
| ATOM | 2473 | CD2 | LEU | A | 316 | 13.784 | 26.387 | 66.501 | 1.00 | 15.84 |
| ATOM | 2474 | N   | ASN | A | 317 | 13.910 | 31.597 | 65.215 | 1.00 | 15.84 |
| ATOM | 2475 | CA  | ASN | A | 317 | 14.312 | 32.673 | 64.360 | 1.00 | 15.91 |
| ATOM | 2476 | C   | ASN | A | 317 | 15.543 | 33.378 | 64.907 | 1.00 | 22.96 |
| ATOM | 2477 | O   | ASN | A | 317 | 16.551 | 33.551 | 64.224 | 1.00 | 27.92 |
| ATOM | 2478 | CB  | ASN | A | 317 | 13.208 | 33.748 | 64.217 | 1.00 | 19.46 |
| ATOM | 2479 | CG  | ASN | A | 317 | 12.179 | 33.441 | 63.147 | 1.00 | 27.63 |
| ATOM | 2480 | OD1 | ASN | A | 317 | 11.822 | 32.273 | 62.889 | 1.00 | 24.23 |
| ATOM | 2481 | ND2 | ASN | A | 317 | 11.664 | 34.504 | 62.541 | 1.00 | 14.06 |
| ATOM | 2482 | N   | GLU | A | 318 | 15.430 | 33.801 | 66.155 | 1.00 | 17.32 |
| ATOM | 2483 | CA  | GLU | A | 318 | 16.489 | 34.567 | 66.808 | 1.00 | 15.82 |
| ATOM | 2484 | C   | GLU | A | 318 | 17.736 | 33.817 | 67.229 | 1.00 | 19.24 |
| ATOM | 2485 | O   | GLU | A | 318 | 18.843 | 34.264 | 66.959 | 1.00 | 19.69 |
| ATOM | 2486 | CB  | GLU | A | 318 | 15.966 | 35.546 | 67.890 | 1.00 | 14.50 |
| ATOM | 2487 | CG  | GLU | A | 318 | 14.904 | 36.470 | 67.308 | 1.00 | 16.88 |
| ATOM | 2488 | CD  | GLU | A | 318 | 15.432 | 37.337 | 66.197 | 1.00 | 20.90 |
| ATOM | 2489 | OE1 | GLU | A | 318 | 16.619 | 37.552 | 66.002 | 1.00 | 17.90 |
| ATOM | 2490 | OE2 | GLU | A | 318 | 14.481 | 37.883 | 65.486 | 1.00 | 20.95 |
| ATOM | 2491 | N   | GLY | A | 319 | 17.556 | 32.693 | 67.913 | 1.00 | 15.48 |
| ATOM | 2492 | CA  | GLY | A | 319 | 18.708 | 31.954 | 68.353 | 1.00 | 13.87 |
| ATOM | 2493 | C   | GLY | A | 319 | 19.645 | 31.601 | 67.227 | 1.00 | 15.36 |
| ATOM | 2494 | O   | GLY | A | 319 | 20.826 | 31.897 | 67.274 | 1.00 | 18.04 |
| ATOM | 2495 | N   | HIS | A | 320 | 19.124 | 30.919 | 66.223 | 1.00 | 16.60 |
| ATOM | 2496 | CA  | HIS | A | 320 | 19.938 | 30.512 | 65.119 | 1.00 | 19.46 |
| ATOM | 2497 | C   | HIS | A | 320 | 20.609 | 31.698 | 64.432 | 1.00 | 19.78 |
| ATOM | 2498 | O   | HIS | A | 320 | 21.721 | 31.601 | 63.957 | 1.00 | 18.89 |
| ATOM | 2499 | CB  | HIS | A | 320 | 19.103 | 29.719 | 64.090 | 1.00 | 21.04 |
| ATOM | 2500 | CG  | HIS | A | 320 | 18.719 | 28.404 | 64.640 | 1.00 | 23.23 |
| ATOM | 2501 | ND1 | HIS | A | 320 | 17.638 | 28.280 | 65.470 | 1.00 | 23.89 |
| ATOM | 2502 | CD2 | HIS | A | 320 | 19.295 | 27.187 | 64.491 | 1.00 | 27.03 |
| ATOM | 2503 | CE1 | HIS | A | 320 | 17.573 | 26.996 | 65.803 | 1.00 | 25.85 |
| ATOM | 2504 | NE2 | HIS | A | 320 | 18.546 | 26.309 | 65.223 | 1.00 | 26.09 |
| ATOM | 2505 | N   | THR | A | 321 | 19.880 | 32.798 | 64.361 | 1.00 | 17.39 |
| ATOM | 2506 | CA  | THR | A | 321 | 20.399 | 34.005 | 63.744 | 1.00 | 17.58 |
| ATOM | 2507 | C   | THR | A | 321 | 21.565 | 34.584 | 64.573 | 1.00 | 20.48 |
| ATOM | 2508 | O   | THR | A | 321 | 22.605 | 34.963 | 64.022 | 1.00 | 17.45 |
| ATOM | 2509 | CB  | THR | A | 321 | 19.301 | 35.065 | 63.457 | 1.00 | 22.10 |
| ATOM | 2510 | OG1 | THR | A | 321 | 18.319 | 34.491 | 62.600 | 1.00 | 17.40 |
| ATOM | 2511 | CG2 | THR | A | 321 | 19.936 | 36.287 | 62.748 | 1.00 | 20.37 |
| ATOM | 2512 | N   | VAL | A | 322 | 21.413 | 34.634 | 65.910 | 1.00 | 14.96 |
| ATOM | 2513 | CA  | VAL | A | 322 | 22.519 | 35.159 | 66.699 | 1.00 | 14.94 |
| ATOM | 2514 | C   | VAL | A | 322 | 23.695 | 34.220 | 66.563 | 1.00 | 17.53 |
| ATOM | 2515 | O   | VAL | A | 322 | 24.843 | 34.611 | 66.518 | 1.00 | 17.42 |
| ATOM | 2516 | CB  | VAL | A | 322 | 22.126 | 35.294 | 68.160 | 1.00 | 17.37 |
| ATOM | 2517 | CG1 | VAL | A | 322 | 23.359 | 35.613 | 68.986 | 1.00 | 13.17 |
| ATOM | 2518 | CG2 | VAL | A | 322 | 21.098 | 36.428 | 68.277 | 1.00 | 17.93 |
| ATOM | 2519 | N   | TYR | A | 323 | 23.383 | 32.948 | 66.490 | 1.00 | 16.41 |
| ATOM | 2520 | CA  | TYR | A | 323 | 24.419 | 31.949 | 66.340 | 1.00 | 14.67 |
| ATOM | 2521 | C   | TYR | A | 323 | 25.190 | 32.191 | 65.026 | 1.00 | 20.23 |
| ATOM | 2522 | O   | TYR | A | 323 | 26.409 | 32.217 | 64.981 | 1.00 | 18.57 |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 2523 | CB  | TYR | A | 323 | 23.837 | 30.513 | 66.424 | 1.00 | 15.23 |
| ATOM | 2524 | CG  | TYR | A | 323 | 24.896 | 29.441 | 66.345 | 1.00 | 16.06 |
| ATOM | 2525 | CD1 | TYR | A | 323 | 25.625 | 29.053 | 67.470 | 1.00 | 17.96 |
| ATOM | 2526 | CD2 | TYR | A | 323 | 25.192 | 28.824 | 65.127 | 1.00 | 20.62 |
| ATOM | 2527 | CE1 | TYR | A | 323 | 26.605 | 28.053 | 67.412 | 1.00 | 15.34 |
| ATOM | 2528 | CE2 | TYR | A | 323 | 26.178 | 27.832 | 65.041 | 1.00 | 21.18 |
| ATOM | 2529 | CZ  | TYR | A | 323 | 26.895 | 27.464 | 66.179 | 1.00 | 19.73 |
| ATOM | 2530 | OH  | TYR | A | 323 | 27.885 | 26.526 | 66.061 | 1.00 | 21.45 |
| ATOM | 2531 | N   | LEU | A | 324 | 24.487 | 32.379 | 63.931 | 1.00 | 17.19 |
| ATOM | 2532 | CA  | LEU | A | 324 | 25.195 | 32.589 | 62.676 | 1.00 | 18.47 |
| ATOM | 2533 | C   | LEU | A | 324 | 25.999 | 33.872 | 62.689 | 1.00 | 21.76 |
| ATOM | 2534 | O   | LEU | A | 324 | 27.157 | 33.935 | 62.279 | 1.00 | 22.47 |
| ATOM | 2535 | CB  | LEU | A | 324 | 24.193 | 32.667 | 61.520 | 1.00 | 20.23 |
| ATOM | 2536 | CG  | LEU | A | 324 | 23.731 | 31.312 | 61.056 | 1.00 | 28.87 |
| ATOM | 2537 | CD1 | LEU | A | 324 | 22.759 | 31.483 | 59.871 | 1.00 | 30.72 |
| ATOM | 2538 | CD2 | LEU | A | 324 | 24.967 | 30.478 | 60.695 | 1.00 | 33.05 |
| ATOM | 2539 | N   | GLU | A | 325 | 25.325 | 34.904 | 63.159 | 1.00 | 19.91 |
| ATOM | 2540 | CA  | GLU | A | 325 | 25.862 | 36.253 | 63.276 | 1.00 | 17.98 |
| ATOM | 2541 | C   | GLU | A | 325 | 27.202 | 36.228 | 63.919 | 1.00 | 20.70 |
| ATOM | 2542 | O   | GLU | A | 325 | 28.138 | 36.847 | 63.449 | 1.00 | 19.47 |
| ATOM | 2543 | CB  | GLU | A | 325 | 24.936 | 37.093 | 64.193 | 1.00 | 19.51 |
| ATOM | 2544 | CG  | GLU | A | 325 | 25.593 | 38.353 | 64.806 | 1.00 | 26.53 |
| ATOM | 2545 | CD  | GLU | A | 325 | 24.735 | 38.992 | 65.891 | 1.00 | 56.58 |
| ATOM | 2546 | OE1 | GLU | A | 325 | 23.578 | 38.680 | 66.153 | 1.00 | 24.74 |
| ATOM | 2547 | OE2 | GLU | A | 325 | 25.351 | 39.940 | 66.533 | 1.00 | 33.68 |
| ATOM | 2548 | N   | ARG | A | 326 | 27.251 | 35.502 | 65.025 | 1.00 | 17.27 |
| ATOM | 2549 | CA  | ARG | A | 326 | 28.462 | 35.384 | 65.802 | 1.00 | 17.75 |
| ATOM | 2550 | C   | ARG | A | 326 | 29.571 | 34.629 | 65.073 | 1.00 | 22.32 |
| ATOM | 2551 | O   | ARG | A | 326 | 30.759 | 34.898 | 65.254 | 1.00 | 18.58 |
| ATOM | 2552 | CB  | ARG | A | 326 | 28.152 | 34.891 | 67.208 | 1.00 | 18.45 |
| ATOM | 2553 | CG  | ARG | A | 326 | 27.526 | 36.021 | 67.998 | 1.00 | 11.87 |
| ATOM | 2554 | CD  | ARG | A | 326 | 27.436 | 35.786 | 69.497 | 1.00 | 18.68 |
| ATOM | 2555 | NE  | ARG | A | 326 | 26.686 | 36.906 | 70.068 | 1.00 | 16.96 |
| ATOM | 2556 | CZ  | ARG | A | 326 | 25.802 | 36.826 | 71.031 | 1.00 | 18.50 |
| ATOM | 2557 | NH1 | ARG | A | 326 | 25.522 | 35.695 | 71.654 | 1.00 | 15.65 |
| ATOM | 2558 | NH2 | ARG | A | 326 | 25.195 | 37.944 | 71.411 | 1.00 | 23.44 |
| ATOM | 2559 | N   | HIS | A | 327 | 29.177 | 33.680 | 64.226 | 1.00 | 21.05 |
| ATOM | 2560 | CA  | HIS | A | 327 | 30.146 | 32.930 | 63.416 | 1.00 | 20.50 |
| ATOM | 2561 | C   | HIS | A | 327 | 30.717 | 33.852 | 62.329 | 1.00 | 23.94 |
| ATOM | 2562 | O   | HIS | A | 327 | 31.910 | 33.810 | 62.042 | 1.00 | 21.92 |
| ATOM | 2563 | CB  | HIS | A | 327 | 29.514 | 31.692 | 62.771 | 1.00 | 19.66 |
| ATOM | 2564 | CG  | HIS | A | 327 | 29.746 | 30.486 | 63.608 | 1.00 | 23.28 |
| ATOM | 2565 | ND1 | HIS | A | 327 | 31.026 | 30.094 | 63.976 | 1.00 | 25.05 |
| ATOM | 2566 | CD2 | HIS | A | 327 | 28.854 | 29.603 | 64.142 | 1.00 | 24.87 |
| ATOM | 2567 | CE1 | HIS | A | 327 | 30.891 | 28.990 | 64.707 | 1.00 | 25.38 |
| ATOM | 2568 | NE2 | HIS | A | 327 | 29.599 | 28.662 | 64.827 | 1.00 | 25.90 |
| ATOM | 2569 | N   | ILE | A | 328 | 29.841 | 34.698 | 61.739 | 1.00 | 17.81 |
| ATOM | 2570 | CA  | ILE | A | 328 | 30.286 | 35.640 | 60.721 | 1.00 | 17.61 |
| ATOM | 2571 | C   | ILE | A | 328 | 31.360 | 36.536 | 61.324 | 1.00 | 26.22 |
| ATOM | 2572 | O   | ILE | A | 328 | 32.473 | 36.706 | 60.805 | 1.00 | 27.90 |
| ATOM | 2573 | CB  | ILE | A | 328 | 29.158 | 36.521 | 60.172 | 1.00 | 19.15 |
| ATOM | 2574 | CG1 | ILE | A | 328 | 28.134 | 35.720 | 59.335 | 1.00 | 20.77 |
| ATOM | 2575 | CG2 | ILE | A | 328 | 29.734 | 37.649 | 59.333 | 1.00 | 16.84 |
| ATOM | 2576 | CD1 | ILE | A | 328 | 26.898 | 36.522 | 58.865 | 1.00 | 15.83 |
| ATOM | 2577 | N   | CYS | A | 329 | 31.005 | 37.125 | 62.446 | 1.00 | 22.11 |
| ATOM | 2578 | CA  | CYS | A | 329 | 31.914 | 37.983 | 63.115 | 1.00 | 25.86 |
| ATOM | 2579 | C   | CYS | A | 329 | 33.169 | 37.244 | 63.548 | 1.00 | 25.73 |
| ATOM | 2580 | O   | CYS | A | 329 | 34.260 | 37.798 | 63.593 | 1.00 | 22.37 |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 2581 | CB  | CYS | A | 329 | 31.209 | 38.714 | 64.264 | 1.00 | 32.85 |
| ATOM | 2582 | SG  | CYS | A | 329 | 30.072 | 40.005 | 63.644 | 1.00 | 40.78 |
| ATOM | 2583 | N   | GLY | A | 330 | 33.018 | 35.970 | 63.905 | 1.00 | 25.01 |
| ATOM | 2584 | CA  | GLY | A | 330 | 34.160 | 35.189 | 64.308 | 1.00 | 24.77 |
| ATOM | 2585 | C   | GLY | A | 330 | 35.075 | 34.986 | 63.108 | 1.00 | 29.37 |
| ATOM | 2586 | O   | GLY | A | 330 | 36.297 | 34.999 | 63.254 | 1.00 | 26.53 |
| ATOM | 2587 | N   | ARG | A | 331 | 34.467 | 34.846 | 61.906 | 1.00 | 27.34 |
| ATOM | 2588 | CA  | ARG | A | 331 | 35.260 | 34.674 | 60.685 | 1.00 | 27.23 |
| ATOM | 2589 | C   | ARG | A | 331 | 36.073 | 35.939 | 60.376 | 1.00 | 29.63 |
| ATOM | 2590 | O   | ARG | A | 331 | 37.235 | 35.895 | 59.990 | 1.00 | 30.48 |
| ATOM | 2591 | CB  | ARG | A | 331 | 34.438 | 34.328 | 59.436 | 1.00 | 22.91 |
| ATOM | 2592 | CG  | ARG | A | 331 | 34.006 | 32.889 | 59.354 | 1.00 | 35.75 |
| ATOM | 2593 | CD  | ARG | A | 331 | 34.619 | 32.119 | 58.189 | 1.00 | 40.73 |
| ATOM | 2594 | NE  | ARG | A | 331 | 34.077 | 30.775 | 58.128 | 1.00 | 51.17 |
| ATOM | 2595 | CZ  | ARG | A | 331 | 33.916 | 29.992 | 59.215 | 1.00 | 76.62 |
| ATOM | 2596 | NH1 | ARG | A | 331 | 34.238 | 30.376 | 60.455 | 1.00 | 62.32 |
| ATOM | 2597 | NH2 | ARG | A | 331 | 33.419 | 28.763 | 59.067 | 1.00 | 59.87 |
| ATOM | 2598 | N   | LEU | A | 332 | 35.429 | 37.066 | 60.532 | 1.00 | 24.33 |
| ATOM | 2599 | CA  | LEU | A | 332 | 36.003 | 38.352 | 60.235 | 1.00 | 24.25 |
| ATOM | 2600 | C   | LEU | A | 332 | 37.005 | 38.862 | 61.245 | 1.00 | 28.60 |
| ATOM | 2601 | O   | LEU | A | 332 | 37.967 | 39.475 | 60.856 | 1.00 | 27.13 |
| ATOM | 2602 | CB  | LEU | A | 332 | 34.859 | 39.381 | 60.194 | 1.00 | 26.61 |
| ATOM | 2603 | CG  | LEU | A | 332 | 34.601 | 40.095 | 58.879 | 1.00 | 36.54 |
| ATOM | 2604 | CD1 | LEU | A | 332 | 35.152 | 39.339 | 57.682 | 1.00 | 36.23 |
| ATOM | 2605 | CD2 | LEU | A | 332 | 33.101 | 40.275 | 58.728 | 1.00 | 41.67 |
| ATOM | 2606 | N   | PHE | A | 333 | 36.751 | 38.659 | 62.546 | 1.00 | 24.79 |
| ATOM | 2607 | CA  | PHE | A | 333 | 37.582 | 39.191 | 63.600 | 1.00 | 21.10 |
| ATOM | 2608 | C   | PHE | A | 333 | 38.244 | 38.192 | 64.501 | 1.00 | 27.46 |
| ATOM | 2609 | O   | PHE | A | 333 | 39.012 | 38.603 | 65.373 | 1.00 | 29.51 |
| ATOM | 2610 | CB  | PHE | A | 333 | 36.818 | 40.254 | 64.422 | 1.00 | 22.40 |
| ATOM | 2611 | CG  | PHE | A | 333 | 36.095 | 41.213 | 63.494 | 1.00 | 25.14 |
| ATOM | 2612 | CD1 | PHE | A | 333 | 36.809 | 42.065 | 62.652 | 1.00 | 28.93 |
| ATOM | 2613 | CD2 | PHE | A | 333 | 34.703 | 41.228 | 63.408 | 1.00 | 30.64 |
| ATOM | 2614 | CE1 | PHE | A | 333 | 36.162 | 42.922 | 61.762 | 1.00 | 28.44 |
| ATOM | 2615 | CE2 | PHE | A | 333 | 34.030 | 42.078 | 62.528 | 1.00 | 32.97 |
| ATOM | 2616 | CZ  | PHE | A | 333 | 34.768 | 42.924 | 61.701 | 1.00 | 29.30 |
| ATOM | 2617 | N   | GLY | A | 334 | 37.949 | 36.900 | 64.345 | 1.00 | 19.09 |
| ATOM | 2618 | CA  | GLY | A | 334 | 38.595 | 35.883 | 65.190 | 1.00 | 18.79 |
| ATOM | 2619 | C   | GLY | A | 334 | 37.676 | 35.152 | 66.174 | 1.00 | 25.13 |
| ATOM | 2620 | O   | GLY | A | 334 | 36.715 | 35.726 | 66.682 | 1.00 | 22.90 |
| ATOM | 2621 | N   | GLU | A | 335 | 38.009 | 33.878 | 66.443 | 1.00 | 22.16 |
| ATOM | 2622 | CA  | GLU | A | 335 | 37.257 | 33.042 | 67.365 | 1.00 | 19.70 |
| ATOM | 2623 | C   | GLU | A | 335 | 37.224 |        |        |      |       |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 2639 | N   | PHE | A | 337 | 37.082 | 36.725 | 69.329 | 1.00 | 18.53 |
| ATOM | 2640 | CA  | PHE | A | 337 | 36.039 | 37.711 | 69.359 | 1.00 | 17.21 |
| ATOM | 2641 | C   | PHE | A | 337 | 34.655 | 37.024 | 69.454 | 1.00 | 20.14 |
| ATOM | 2642 | O   | PHE | A | 337 | 33.746 | 37.513 | 70.132 | 1.00 | 20.44 |
| ATOM | 2643 | CB  | PHE | A | 337 | 36.127 | 38.575 | 68.102 | 1.00 | 18.16 |
| ATOM | 2644 | CG  | PHE | A | 337 | 35.261 | 39.817 | 68.112 | 1.00 | 21.27 |
| ATOM | 2645 | CD1 | PHE | A | 337 | 35.319 | 40.723 | 69.175 | 1.00 | 26.55 |
| ATOM | 2646 | CD2 | PHE | A | 337 | 34.405 | 40.095 | 67.044 | 1.00 | 23.27 |
| ATOM | 2647 | CE1 | PHE | A | 337 | 34.543 | 41.883 | 69.192 | 1.00 | 27.57 |
| ATOM | 2648 | CE2 | PHE | A | 337 | 33.633 | 41.256 | 67.026 | 1.00 | 25.34 |
| ATOM | 2649 | CZ  | PHE | A | 337 | 33.707 | 42.141 | 68.106 | 1.00 | 25.01 |
| ATOM | 2650 | N   | ARG | A | 338 | 34.477 | 35.901 | 68.751 | 1.00 | 14.22 |
| ATOM | 2651 | CA  | ARG | A | 338 | 33.217 | 35.202 | 68.800 | 1.00 | 14.00 |
| ATOM | 2652 | C   | ARG | A | 338 | 32.926 | 34.834 | 70.234 | 1.00 | 20.03 |
| ATOM | 2653 | O   | ARG | A | 338 | 31.809 | 34.975 | 70.702 | 1.00 | 19.54 |
| ATOM | 2654 | CB  | ARG | A | 338 | 33.224 | 33.937 | 67.959 | 1.00 | 17.99 |
| ATOM | 2655 | CG  | ARG | A | 338 | 31.869 | 33.248 | 67.913 | 1.00 | 18.25 |
| ATOM | 2656 | CD  | ARG | A | 338 | 31.813 | 32.116 | 66.876 | 1.00 | 21.97 |
| ATOM | 2657 | NE  | ARG | A | 338 | 32.426 | 30.901 | 67.397 | 1.00 | 16.11 |
| ATOM | 2658 | CZ  | ARG | A | 338 | 31.790 | 29.798 | 67.805 | 1.00 | 23.47 |
| ATOM | 2659 | NH1 | ARG | A | 338 | 30.473 | 29.632 | 67.750 | 1.00 | 18.92 |
| ATOM | 2660 | NH2 | ARG | A | 338 | 32.514 | 28.791 | 68.274 | 1.00 | 21.62 |
| ATOM | 2661 | N   | HIS | A | 339 | 33.937 | 34.373 | 70.942 | 1.00 | 14.98 |
| ATOM | 2662 | CA  | HIS | A | 339 | 33.723 | 33.987 | 72.330 | 1.00 | 16.26 |
| ATOM | 2663 | C   | HIS | A | 339 | 33.365 | 35.174 | 73.245 | 1.00 | 17.16 |
| ATOM | 2664 | O   | HIS | A | 339 | 32.516 | 35.096 | 74.153 | 1.00 | 14.74 |
| ATOM | 2665 | CB  | HIS | A | 339 | 34.928 | 33.190 | 72.871 | 1.00 | 16.32 |
| ATOM | 2666 | CG  | HIS | A | 339 | 34.831 | 31.770 | 72.472 | 1.00 | 18.27 |
| ATOM | 2667 | ND1 | HIS | A | 339 | 34.797 | 30.768 | 73.418 | 1.00 | 20.08 |
| ATOM | 2668 | CD2 | HIS | A | 339 | 34.764 | 31.220 | 71.243 | 1.00 | 20.71 |
| ATOM | 2669 | CE1 | HIS | A | 339 | 34.709 | 29.622 | 72.759 | 1.00 | 20.27 |
| ATOM | 2670 | NE2 | HIS | A | 339 | 34.673 | 29.865 | 71.458 | 1.00 | 21.30 |
| ATOM | 2671 | N   | PHE | A | 340 | 34.014 | 36.275 | 72.957 | 1.00 | 12.98 |
| ATOM | 2672 | CA  | PHE | A | 340 | 33.817 | 37.499 | 73.664 | 1.00 | 14.03 |
| ATOM | 2673 | C   | PHE | A | 340 | 32.362 | 37.955 | 73.510 | 1.00 | 19.81 |
| ATOM | 2674 | O   | PHE | A | 340 | 31.671 | 38.339 | 74.478 | 1.00 | 17.18 |
| ATOM | 2675 | CB  | PHE | A | 340 | 34.807 | 38.566 | 73.162 | 1.00 | 14.06 |
| ATOM | 2676 | CG  | PHE | A | 340 | 34.520 | 39.960 | 73.671 | 1.00 | 16.25 |
| ATOM | 2677 | CD1 | PHE | A | 340 | 34.983 | 40.378 | 74.921 | 1.00 | 14.61 |
| ATOM | 2678 | CD2 | PHE | A | 340 | 33.804 | 40.871 | 72.889 | 1.00 | 20.48 |
| ATOM | 2679 | CE1 | PHE | A | 340 | 34.738 | 41.654 | 75.420 | 1.00 | 11.01 |
| ATOM | 2680 | CE2 | PHE | A | 340 | 33.545 | 42.161 | 73.362 | 1.00 | 21.48 |
| ATOM | 2681 | CZ  | PHE | A | 340 | 34.016 | 42.53  |        |      |       |



|      |      |     |           |        |        |        |      |       |
|------|------|-----|-----------|--------|--------|--------|------|-------|
| ATOM | 2697 | C   | LEU A 343 | 29.145 | 37.001 | 77.172 | 1.00 | 15.26 |
| ATOM | 2698 | O   | LEU A 343 | 28.437 | 36.987 | 78.144 | 1.00 | 17.28 |
| ATOM | 2699 | CB  | LEU A 343 | 31.338 | 35.830 | 77.389 | 1.00 | 14.50 |
| ATOM | 2700 | CG  | LEU A 343 | 31.392 | 35.853 | 78.888 | 1.00 | 19.65 |
| ATOM | 2701 | CD1 | LEU A 343 | 30.614 | 34.660 | 79.473 | 1.00 | 19.94 |
| ATOM | 2702 | CD2 | LEU A 343 | 32.862 | 35.680 | 79.227 | 1.00 | 19.54 |
| ATOM | 2703 | N   | GLY A 344 | 29.269 | 38.039 | 76.392 | 1.00 | 13.33 |
| ATOM | 2704 | CA  | GLY A 344 | 28.516 | 39.252 | 76.617 | 1.00 | 13.13 |
| ATOM | 2705 | C   | GLY A 344 | 26.993 | 38.975 | 76.424 | 1.00 | 17.09 |
| ATOM | 2706 | O   | GLY A 344 | 26.209 | 39.525 | 77.181 | 1.00 | 18.43 |
| ATOM | 2707 | N   | GLY A 345 | 26.603 | 38.115 | 75.431 | 1.00 | 15.02 |
| ATOM | 2708 | CA  | GLY A 345 | 25.228 | 37.703 | 75.168 | 1.00 | 12.69 |
| ATOM | 2709 | C   | GLY A 345 | 24.699 | 37.028 | 76.459 | 1.00 | 19.95 |
| ATOM | 2710 | O   | GLY A 345 | 23.583 | 37.271 | 76.883 | 1.00 | 19.12 |
| ATOM | 2711 | N   | TRP A 346 | 25.515 | 36.189 | 77.135 | 1.00 | 16.29 |
| ATOM | 2712 | CA  | TRP A 346 | 25.126 | 35.535 | 78.389 | 1.00 | 14.14 |
| ATOM | 2713 | C   | TRP A 346 | 24.797 | 36.599 | 79.432 | 1.00 | 22.96 |
| ATOM | 2714 | O   | TRP A 346 | 23.812 | 36.495 | 80.202 | 1.00 | 17.35 |
| ATOM | 2715 | CB  | TRP A 346 | 26.221 | 34.583 | 78.935 | 1.00 | 13.13 |
| ATOM | 2716 | CG  | TRP A 346 | 25.805 | 33.923 | 80.234 | 1.00 | 15.08 |
| ATOM | 2717 | CD1 | TRP A 346 | 26.003 | 34.405 | 81.508 | 1.00 | 16.98 |
| ATOM | 2718 | CD2 | TRP A 346 | 25.091 | 32.675 | 80.386 | 1.00 | 15.17 |
| ATOM | 2719 | NE1 | TRP A 346 | 25.469 | 33.520 | 82.420 | 1.00 | 16.47 |
| ATOM | 2720 | CE2 | TRP A 346 | 24.903 | 32.462 | 81.769 | 1.00 | 17.52 |
| ATOM | 2721 | CE3 | TRP A 346 | 24.593 | 31.728 | 79.481 | 1.00 | 15.86 |
| ATOM | 2722 | CZ2 | TRP A 346 | 24.228 | 31.326 | 82.257 | 1.00 | 16.80 |
| ATOM | 2723 | CZ3 | TRP A 346 | 23.949 | 30.619 | 79.970 | 1.00 | 17.27 |
| ATOM | 2724 | CH2 | TRP A 346 | 23.761 | 30.427 | 81.347 | 1.00 | 17.06 |
| ATOM | 2725 | N   | GLY A 347 | 25.620 | 37.668 | 79.449 | 1.00 | 15.29 |
| ATOM | 2726 | CA  | GLY A 347 | 25.395 | 38.744 | 80.397 | 1.00 | 13.67 |
| ATOM | 2727 | C   | GLY A 347 | 24.083 | 39.473 | 80.141 | 1.00 | 17.65 |
| ATOM | 2728 | O   | GLY A 347 | 23.415 | 39.859 | 81.083 | 1.00 | 18.50 |
| ATOM | 2729 | N   | GLU A 348 | 23.728 | 39.660 | 78.868 | 1.00 | 16.50 |
| ATOM | 2730 | CA  | GLU A 348 | 22.474 | 40.310 | 78.494 | 1.00 | 16.15 |
| ATOM | 2731 | C   | GLU A 348 | 21.306 | 39.438 | 78.939 | 1.00 | 16.51 |
| ATOM | 2732 | O   | GLU A 348 | 20.259 | 39.922 | 79.420 | 1.00 | 15.73 |
| ATOM | 2733 | CB  | GLU A 348 | 22.445 | 40.591 | 76.996 | 1.00 | 17.40 |
| ATOM | 2734 | CG  | GLU A 348 | 23.386 | 41.764 | 76.683 | 1.00 | 24.32 |
| ATOM | 2735 | CD  | GLU A 348 | 22.918 | 43.017 | 77.378 | 1.00 | 50.61 |
| ATOM | 2736 | OE1 | GLU A 348 | 21.754 | 43.390 | 77.378 | 1.00 | 54.41 |
| ATOM | 2737 | OE2 | GLU A 348 | 23.877 | 43.633 | 78.016 | 1.00 | 27.35 |
| ATOM | 2738 | N   | LEU A 349 | 21.525 | 38.115 | 78.807 | 1.00 | 14.77 |
| ATOM | 2739 | CA  | LEU A 349 | 20.541 | 37.132 | 79.269 | 1.00 | 16.97 |
| ATOM | 2740 | C   | LEU A 349 | 20.329 | 37.268 | 80.814 | 1.00 | 19.32 |
| ATOM | 2741 | O   | LEU A 349 | 19.193 | 37.312 | 81.286 | 1.00 | 17.99 |
| ATOM | 2742 | CB  | LEU A 349 | 20.915 | 35.681 | 78.924 | 1.00 | 15.80 |
| ATOM | 2743 | CG  | LEU A 349 | 19.824 | 34.699 | 79.338 | 1.00 | 19.63 |
| ATOM | 2744 | CD1 | LEU A 349 | 18.534 | 34.994 | 78.565 | 1.00 | 17.40 |
| ATOM | 2745 | CD2 | LEU A 349 | 20.304 | 33.265 | 79.088 | 1.00 | 21.23 |
| ATOM | 2746 | N   | GLN A 350 | 21.405 | 37.344 | 81.603 | 1.00 | 11.38 |
| ATOM | 2747 | CA  | GLN A 350 | 21.262 | 37.507 | 83.026 | 1.00 | 13.30 |
| ATOM | 2748 | C   | GLN A 350 | 20.449 | 38.753 | 83.318 | 1.00 | 22.11 |
| ATOM | 2749 | O   | GLN A 350 | 19.613 | 38.805 | 84.221 | 1.00 | 23.26 |
| ATOM | 2750 | CB  | GLN A 350 | 22.637 | 37.748 | 83.635 | 1.00 | 17.68 |
| ATOM | 2751 | CG  | GLN A 350 | 23.590 | 36.553 | 83.432 | 1.00 | 17.78 |
| ATOM | 2752 | CD  | GLN A 350 | 24.971 | 36.862 | 84.006 | 1.00 | 21.19 |
| ATOM | 2753 | OE1 | GLN A 350 | 25.561 | 36.059 | 84.728 | 1.00 | 29.39 |
| ATOM | 2754 | NE2 | GLN A 350 | 25.485 | 38.043 | 83.712 | 1.00 | 20.71 |



|      |      |     |           |        |        |        |      |       |
|------|------|-----|-----------|--------|--------|--------|------|-------|
| ATOM | 2755 | N   | ASN A 351 | 20.711 | 39.786 | 82.539 | 1.00 | 16.08 |
| ATOM | 2756 | CA  | ASN A 351 | 20.019 | 41.023 | 82.694 | 1.00 | 15.68 |
| ATOM | 2757 | C   | ASN A 351 | 18.530 | 40.851 | 82.433 | 1.00 | 22.65 |
| ATOM | 2758 | O   | ASN A 351 | 17.688 | 41.307 | 83.234 | 1.00 | 18.44 |
| ATOM | 2759 | CB  | ASN A 351 | 20.577 | 42.095 | 81.736 | 1.00 | 18.73 |
| ATOM | 2760 | CG  | ASN A 351 | 21.934 | 42.637 | 82.197 | 1.00 | 14.85 |
| ATOM | 2761 | OD1 | ASN A 351 | 22.426 | 42.257 | 83.267 | 1.00 | 23.05 |
| ATOM | 2762 | ND2 | ASN A 351 | 22.551 | 43.464 | 81.352 | 1.00 | 19.82 |
| ATOM | 2763 | N   | SER A 352 | 18.195 | 40.218 | 81.299 | 1.00 | 17.59 |
| ATOM | 2764 | CA  | SER A 352 | 16.788 | 40.020 | 80.979 | 1.00 | 16.98 |
| ATOM | 2765 | C   | SER A 352 | 16.077 | 39.199 | 82.034 | 1.00 | 19.09 |
| ATOM | 2766 | O   | SER A 352 | 14.907 | 39.453 | 82.392 | 1.00 | 21.78 |
| ATOM | 2767 | CB  | SER A 352 | 16.621 | 39.355 | 79.633 | 1.00 | 25.92 |
| ATOM | 2768 | OG  | SER A 352 | 16.959 | 40.271 | 78.629 | 1.00 | 39.51 |
| ATOM | 2769 | N   | VAL A 353 | 16.788 | 38.181 | 82.510 | 1.00 | 15.36 |
| ATOM | 2770 | CA  | VAL A 353 | 16.243 | 37.318 | 83.544 | 1.00 | 16.80 |
| ATOM | 2771 | C   | VAL A 353 | 15.963 | 38.106 | 84.810 | 1.00 | 23.73 |
| ATOM | 2772 | O   | VAL A 353 | 14.900 | 37.966 | 85.420 | 1.00 | 19.97 |
| ATOM | 2773 | CB  | VAL A 353 | 17.083 | 36.073 | 83.808 | 1.00 | 18.09 |
| ATOM | 2774 | CG1 | VAL A 353 | 16.540 | 35.288 | 84.989 | 1.00 | 18.20 |
| ATOM | 2775 | CG2 | VAL A 353 | 17.021 | 35.169 | 82.571 | 1.00 | 19.40 |
| ATOM | 2776 | N   | LYS A 354 | 16.930 | 38.952 | 85.184 | 1.00 | 19.41 |
| ATOM | 2777 | CA  | LYS A 354 | 16.804 | 39.739 | 86.375 | 1.00 | 18.40 |
| ATOM | 2778 | C   | LYS A 354 | 15.648 | 40.702 | 86.261 | 1.00 | 25.72 |
| ATOM | 2779 | O   | LYS A 354 | 14.806 | 40.856 | 87.147 | 1.00 | 23.94 |
| ATOM | 2780 | CB  | LYS A 354 | 18.090 | 40.464 | 86.695 | 1.00 | 25.22 |
| ATOM | 2781 | CG  | LYS A 354 | 18.027 | 41.168 | 88.047 | 1.00 | 42.11 |
| ATOM | 2782 | CD  | LYS A 354 | 19.202 | 42.103 | 88.264 | 1.00 | 54.17 |
| ATOM | 2783 | CE  | LYS A 354 | 19.258 | 42.717 | 89.654 | 1.00 | 46.55 |
| ATOM | 2784 | NZ  | LYS A 354 | 20.438 | 43.583 | 89.846 | 1.00 | 64.93 |
| ATOM | 2785 | N   | THR A 355 | 15.596 | 41.356 | 85.140 | 1.00 | 21.59 |
| ATOM | 2786 | CA  | THR A 355 | 14.538 | 42.307 | 84.882 | 1.00 | 21.16 |
| ATOM | 2787 | C   | THR A 355 | 13.127 | 41.703 | 85.000 | 1.00 | 26.96 |
| ATOM | 2788 | O   | THR A 355 | 12.280 | 42.192 | 85.741 | 1.00 | 21.59 |
| ATOM | 2789 | CB  | THR A 355 | 14.786 | 42.962 | 83.520 | 1.00 | 26.90 |
| ATOM | 2790 | OG1 | THR A 355 | 15.896 | 43.824 | 83.628 | 1.00 | 29.56 |
| ATOM | 2791 | CG2 | THR A 355 | 13.546 | 43.707 | 83.039 | 1.00 | 41.34 |
| ATOM | 2792 | N   | PHE A 356 | 12.855 | 40.607 | 84.285 | 1.00 | 22.14 |
| ATOM | 2793 | CA  | PHE A 356 | 11.550 | 39.993 | 84.349 | 1.00 | 18.19 |
| ATOM | 2794 | C   | PHE A 356 | 11.308 | 39.245 | 85.600 | 1.00 | 16.86 |
| ATOM | 2795 | O   | PHE A 356 | 10.177 | 39.093 | 85.989 | 1.00 | 19.45 |
| ATOM | 2796 | CB  | PHE A 356 | 11.490 | 38.867 | 83.333 | 1.00 | 22.01 |
| ATOM | 2797 | CG  | PHE A 356 | 11.175 | 39.327 | 81.967 | 1.00 | 24.96 |
| ATOM | 2798 | CD1 | PHE A 356 | 10.016 | 40.069 | 81.747 | 1.00 | 31.09 |
| ATOM | 2799 | CD2 | PHE A 356 | 11.992 | 38.977 | 80.890 | 1.00 | 27.87 |
| ATOM | 2800 | CE1 | PHE A 356 | 9.686  | 40.514 | 80.466 | 1.00 | 34.87 |
| ATOM | 2801 | CE2 | PHE A 356 | 11.658 | 39.390 | 79.598 | 1.00 | 35.46 |
| ATOM | 2802 | CZ  | PHE A 356 | 10.509 | 40.161 | 79.391 | 1.00 | 36.07 |
| ATOM | 2803 | N   | GLY A 357 | 12.355 | 38.671 | 86.149 | 1.00 | 13.91 |
| ATOM | 2804 | CA  | GLY A 357 | 12.250 | 37.789 | 87.324 | 1.00 | 14.94 |
| ATOM | 2805 | C   | GLY A 357 | 12.506 | 36.315 | 86.859 | 1.00 | 18.85 |
| ATOM | 2806 | O   | GLY A 357 | 12.081 | 35.910 | 85.757 | 1.00 | 20.96 |
| ATOM | 2807 | N   | GLU A 358 | 13.188 | 35.511 | 87.690 | 1.00 | 14.21 |
| ATOM | 2808 | CA  | GLU A 358 | 13.548 | 34.176 | 87.315 | 1.00 | 18.10 |
| ATOM | 2809 | C   | GLU A 358 | 12.406 | 33.208 | 87.139 | 1.00 | 22.35 |
| ATOM | 2810 | O   | GLU A 358 | 12.594 | 32.093 | 86.599 | 1.00 | 18.73 |
| ATOM | 2811 | CB  | GLU A 358 | 14.620 | 33.586 | 88.215 | 1.00 | 20.85 |
| ATOM | 2812 | CG  | GLU A 358 | 14.021 | 33.077 | 89.527 | 1.00 | 35.73 |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 2813 | CD  | GLU | A | 358 | 15.008 | 33.053 | 90.661 | 1.00 | 64.53 |
| ATOM | 2814 | OE1 | GLU | A | 358 | 16.138 | 32.655 | 90.520 | 1.00 | 38.29 |
| ATOM | 2815 | OE2 | GLU | A | 358 | 14.517 | 33.496 | 91.801 | 1.00 | 89.00 |
| ATOM | 2816 | N   | THR | A | 359 | 11.222 | 33.608 | 87.576 | 1.00 | 16.44 |
| ATOM | 2817 | CA  | THR | A | 359 | 10.112 | 32.687 | 87.414 | 1.00 | 17.09 |
| ATOM | 2818 | C   | THR | A | 359 | 9.142  | 33.199 | 86.407 | 1.00 | 18.44 |
| ATOM | 2819 | O   | THR | A | 359 | 8.076  | 32.662 | 86.290 | 1.00 | 19.27 |
| ATOM | 2820 | CB  | THR | A | 359 | 9.359  | 32.432 | 88.713 | 1.00 | 21.12 |
| ATOM | 2821 | OG1 | THR | A | 359 | 8.721  | 33.635 | 89.097 | 1.00 | 20.02 |
| ATOM | 2822 | CG2 | THR | A | 359 | 10.295 | 31.956 | 89.804 | 1.00 | 20.69 |
| ATOM | 2823 | N   | HIS | A | 360 | 9.516  | 34.245 | 85.712 | 1.00 | 13.71 |
| ATOM | 2824 | CA  | HIS | A | 360 | 8.666  | 34.841 | 84.723 | 1.00 | 14.97 |
| ATOM | 2825 | C   | HIS | A | 360 | 8.553  | 33.974 | 83.467 | 1.00 | 20.83 |
| ATOM | 2826 | O   | HIS | A | 360 | 9.543  | 33.532 | 82.898 | 1.00 | 18.41 |
| ATOM | 2827 | CB  | HIS | A | 360 | 9.171  | 36.224 | 84.380 | 1.00 | 16.95 |
| ATOM | 2828 | CG  | HIS | A | 360 | 8.149  | 36.963 | 83.639 | 1.00 | 19.78 |
| ATOM | 2829 | ND1 | HIS | A | 360 | 7.496  | 38.077 | 84.178 | 1.00 | 23.17 |
| ATOM | 2830 | CD2 | HIS | A | 360 | 7.657  | 36.712 | 82.406 | 1.00 | 21.01 |
| ATOM | 2831 | CE1 | HIS | A | 360 | 6.622  | 38.481 | 83.251 | 1.00 | 22.01 |
| ATOM | 2832 | NE2 | HIS | A | 360 | 6.711  | 37.664 | 82.171 | 1.00 | 24.05 |
| ATOM | 2833 | N   | PRO | A | 361 | 7.318  | 33.722 | 83.043 | 1.00 | 21.94 |
| ATOM | 2834 | CA  | PRO | A | 361 | 7.096  | 32.895 | 81.876 | 1.00 | 21.68 |
| ATOM | 2835 | C   | PRO | A | 361 | 7.728  | 33.450 | 80.602 | 1.00 | 23.08 |
| ATOM | 2836 | O   | PRO | A | 361 | 7.928  | 32.715 | 79.648 | 1.00 | 19.72 |
| ATOM | 2837 | CB  | PRO | A | 361 | 5.585  | 32.700 | 81.755 | 1.00 | 22.85 |
| ATOM | 2838 | CG  | PRO | A | 361 | 5.027  | 33.012 | 83.134 | 1.00 | 28.59 |
| ATOM | 2839 | CD  | PRO | A | 361 | 6.048  | 33.917 | 83.803 | 1.00 | 21.80 |
| ATOM | 2840 | N   | PHE | A | 362 | 8.055  | 34.731 | 80.582 | 1.00 | 20.70 |
| ATOM | 2841 | CA  | PHE | A | 362 | 8.690  | 35.270 | 79.394 | 1.00 | 22.53 |
| ATOM | 2842 | C   | PHE | A | 362 | 10.150 | 34.915 | 79.350 | 1.00 | 20.33 |
| ATOM | 2843 | O   | PHE | A | 362 | 10.817 | 35.272 | 78.398 | 1.00 | 21.38 |
| ATOM | 2844 | CB  | PHE | A | 362 | 8.534  | 36.768 | 79.124 | 1.00 | 25.38 |
| ATOM | 2845 | CG  | PHE | A | 362 | 7.103  | 37.248 | 79.022 | 1.00 | 28.56 |
| ATOM | 2846 | CD1 | PHE | A | 362 | 6.042  | 36.377 | 78.783 | 1.00 | 29.73 |
| ATOM | 2847 | CD2 | PHE | A | 362 | 6.826  | 38.604 | 79.181 | 1.00 | 29.51 |
| ATOM | 2848 | CE1 | PHE | A | 362 | 4.730  | 36.849 | 78.687 | 1.00 | 29.17 |
| ATOM | 2849 | CE2 | PHE | A | 362 | 5.517  | 39.086 | 79.106 | 1.00 | 32.58 |
| ATOM | 2850 | CZ  | PHE | A | 362 | 4.465  | 38.211 | 78.869 | 1.00 | 27.13 |
| ATOM | 2851 | N   | THR | A | 363 | 10.641 | 34.241 | 80.382 | 1.00 | 17.45 |
| ATOM | 2852 | CA  | THR | A | 363 | 12.032 | 33.825 | 80.375 | 1.00 | 16.26 |
| ATOM | 2853 | C   | THR | A | 363 | 12.190 | 32.400 | 79.820 | 1.00 | 17.12 |
| ATOM | 2854 | O   | THR | A | 363 | 13.271 | 31.848 | 79.771 | 1.00 | 17.12 |
| ATOM | 2855 | CB  | THR | A | 363 | 12.718 | 33.967 | 81.730 | 1.00 | 15.97 |
| ATOM | 2856 | OG1 | THR | A | 363 | 12.001 | 33.241 | 82.735 | 1.00 | 18.45 |
| ATOM | 2857 | CG2 | THR | A | 363 | 12.820 | 35.453 | 82.059 | 1.00 | 13.79 |
| ATOM | 2858 | N   | LYS | A | 364 | 11.100 | 31.782 | 79.410 | 1.00 | 13.55 |
| ATOM | 2859 | CA  | LYS | A | 364 | 11.179 | 30.425 | 78.850 | 1.00 | 12.81 |
| ATOM | 2860 | C   | LYS | A | 364 | 11.607 | 30.536 | 77.406 | 1.00 | 17.59 |
| ATOM | 2861 | O   | LYS | A | 364 | 11.315 | 31.518 | 76.718 | 1.00 | 18.05 |
| ATOM | 2862 | CB  | LYS | A | 364 | 9.807  | 29.741 | 78.851 | 1.00 | 14.15 |
| ATOM | 2863 | CG  | LYS | A | 364 | 9.285  | 29.478 | 80.259 | 1.00 | 22.73 |
| ATOM | 2864 | CD  | LYS | A | 364 | 7.787  | 29.209 | 80.302 | 1.00 | 24.91 |
| ATOM | 2865 | CE  | LYS | A | 364 | 7.322  | 28.851 | 81.703 | 1.00 | 24.87 |
| ATOM | 2866 | NZ  | LYS | A | 364 | 6.143  | 27.983 | 81.688 | 1.00 | 36.58 |
| ATOM | 2867 | N   | LEU | A | 365 | 12.274 | 29.534 | 76.906 | 1.00 | 14.53 |
| ATOM | 2868 | CA  | LEU | A | 365 | 12.667 | 29.596 | 75.511 | 1.00 | 16.17 |
| ATOM | 2869 | C   | LEU | A | 365 | 11.421 | 29.458 | 74.619 | 1.00 | 19.12 |
| ATOM | 2870 | O   | LEU | A | 365 | 11.229 | 30.201 | 73.656 | 1.00 | 19.11 |



6012240-022209

|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 2871 | CB  | LEU | A | 365 | 13.718 | 28.500 | 75.236 | 1.00 | 16.49 |
| ATOM | 2872 | CG  | LEU | A | 365 | 14.458 | 28.603 | 73.913 | 1.00 | 21.42 |
| ATOM | 2873 | CD1 | LEU | A | 365 | 15.106 | 29.973 | 73.789 | 1.00 | 17.49 |
| ATOM | 2874 | CD2 | LEU | A | 365 | 15.537 | 27.525 | 73.929 | 1.00 | 21.26 |
| ATOM | 2875 | N   | VAL | A | 366 | 10.560 | 28.499 | 74.950 | 1.00 | 16.34 |
| ATOM | 2876 | CA  | VAL | A | 366 | 9.318  | 28.315 | 74.230 | 1.00 | 18.86 |
| ATOM | 2877 | C   | VAL | A | 366 | 8.188  | 28.979 | 75.059 | 1.00 | 22.69 |
| ATOM | 2878 | O   | VAL | A | 366 | 7.931  | 28.576 | 76.180 | 1.00 | 21.37 |
| ATOM | 2879 | CB  | VAL | A | 366 | 9.012  | 26.855 | 73.923 | 1.00 | 22.73 |
| ATOM | 2880 | CG1 | VAL | A | 366 | 7.741  | 26.775 | 73.070 | 1.00 | 20.71 |
| ATOM | 2881 | CG2 | VAL | A | 366 | 10.189 | 26.241 | 73.158 | 1.00 | 22.18 |
| ATOM | 2882 | N   | VAL | A | 367 | 7.537  | 30.015 | 74.521 | 1.00 | 20.21 |
| ATOM | 2883 | CA  | VAL | A | 367 | 6.487  | 30.723 | 75.263 | 1.00 | 21.75 |
| ATOM | 2884 | C   | VAL | A | 367 | 5.071  | 30.530 | 74.765 | 1.00 | 31.76 |
| ATOM | 2885 | O   | VAL | A | 367 | 4.818  | 30.099 | 73.637 | 1.00 | 33.07 |
| ATOM | 2886 | CB  | VAL | A | 367 | 6.737  | 32.204 | 75.201 | 1.00 | 24.64 |
| ATOM | 2887 | CG1 | VAL | A | 367 | 8.102  | 32.527 | 75.814 | 1.00 | 23.06 |
| ATOM | 2888 | CG2 | VAL | A | 367 | 6.628  | 32.633 | 73.739 | 1.00 | 25.37 |
| ATOM | 2889 | N   | ASP | A | 368 | 4.134  | 30.913 | 75.631 | 1.00 | 26.47 |
| ATOM | 2890 | CA  | ASP | A | 368 | 2.717  | 30.841 | 75.295 | 1.00 | 24.49 |
| ATOM | 2891 | C   | ASP | A | 368 | 2.203  | 32.251 | 75.126 | 1.00 | 19.48 |
| ATOM | 2892 | O   | ASP | A | 368 | 1.991  | 32.972 | 76.069 | 1.00 | 21.34 |
| ATOM | 2893 | CB  | ASP | A | 368 | 1.904  | 30.081 | 76.365 | 1.00 | 28.12 |
| ATOM | 2894 | CG  | ASP | A | 368 | 0.482  | 29.882 | 75.908 | 1.00 | 37.10 |
| ATOM | 2895 | OD1 | ASP | A | 368 | 0.023  | 30.365 | 74.885 | 1.00 | 30.33 |
| ATOM | 2896 | OD2 | ASP | A | 368 | -0.202 | 29.155 | 76.725 | 1.00 | 34.29 |
| ATOM | 2897 | N   | LEU | A | 369 | 2.046  | 32.675 | 73.915 | 1.00 | 17.90 |
| ATOM | 2898 | CA  | LEU | A | 369 | 1.611  | 34.025 | 73.688 | 1.00 | 19.61 |
| ATOM | 2899 | C   | LEU | A | 369 | 0.107  | 34.208 | 73.712 | 1.00 | 23.98 |
| ATOM | 2900 | O   | LEU | A | 369 | -0.419 | 35.236 | 73.282 | 1.00 | 27.35 |
| ATOM | 2901 | CB  | LEU | A | 369 | 2.202  | 34.607 | 72.383 | 1.00 | 19.83 |
| ATOM | 2902 | CG  | LEU | A | 369 | 3.702  | 34.866 | 72.488 | 1.00 | 24.77 |
| ATOM | 2903 | CD1 | LEU | A | 369 | 4.217  | 35.374 | 71.135 | 1.00 | 20.98 |
| ATOM | 2904 | CD2 | LEU | A | 369 | 3.998  | 35.838 | 73.626 | 1.00 | 23.40 |
| ATOM | 2905 | N   | THR | A | 370 | -0.592 | 33.220 | 74.199 | 1.00 | 22.21 |
| ATOM | 2906 | CA  | THR | A | 370 | -2.033 | 33.349 | 74.254 | 1.00 | 22.43 |
| ATOM | 2907 | C   | THR | A | 370 | -2.440 | 34.563 | 75.093 | 1.00 | 28.86 |
| ATOM | 2908 | O   | THR | A | 370 | -2.147 | 34.665 | 76.295 | 1.00 | 27.57 |
| ATOM | 2909 | CB  | THR | A | 370 | -2.678 | 32.128 | 74.916 | 1.00 | 31.88 |
| ATOM | 2910 | OG1 | THR | A | 370 | -2.352 | 30.960 | 74.212 | 1.00 | 35.39 |
| ATOM | 2911 | CG2 | THR | A | 370 | -4.183 | 32.323 | 74.893 | 1.00 | 34.18 |
| ATOM | 2912 | N   | ASP | A | 371 | -3.130 | 35.489 | 74.439 | 1.00 | 28.25 |
| ATOM | 2913 | CA  | ASP | A | 371 | -3.595 | 36.685 | 75.107 | 1.00 | 27.92 |
| ATOM | 2914 | C   | ASP | A | 371 | -2.498 | 37.603 | 75.529 | 1.00 | 28.33 |
| ATOM | 2915 | O   | ASP | A | 371 | -2.665 | 38.374 | 76.445 | 1.00 | 25.40 |
| ATOM | 2916 | CB  | ASP | A | 371 | -4.508 | 36.369 | 76.293 | 1.00 | 32.10 |
| ATOM | 2917 | CG  | ASP | A | 371 | -5.847 | 35.839 | 75.826 | 1.00 | 46.60 |
| ATOM | 2918 | OD1 | ASP | A | 371 | -6.474 | 36.318 | 74.880 | 1.00 | 45.97 |
| ATOM | 2919 | OD2 | ASP | A | 371 | -6.232 | 34.791 | 76.516 | 1.00 | 45.84 |
| ATOM | 2920 | N   | ILE | A | 372 | -1.389 | 37.540 | 74.841 | 1.00 | 25.39 |
| ATOM | 2921 | CA  | ILE | A | 372 | -0.306 | 38.436 | 75.177 | 1.00 | 24.43 |
| ATOM | 2922 | C   | ILE | A | 372 | 0.113  | 39.165 | 73.929 | 1.00 | 24.31 |
| ATOM | 2923 | O   | ILE | A | 372 | 0.327  | 38.512 | 72.915 | 1.00 | 26.21 |
| ATOM | 2924 | CB  | ILE | A | 372 | 0.879  | 37.637 | 75.654 | 1.00 | 28.18 |
| ATOM | 2925 | CG1 | ILE | A | 372 | 0.606  | 37.086 | 77.045 | 1.00 | 26.69 |
| ATOM | 2926 | CG2 | ILE | A | 372 | 2.092  | 38.554 | 75.644 | 1.00 | 31.78 |
| ATOM | 2927 | CD1 | ILE | A | 372 | 0.652  | 38.193 | 78.085 | 1.00 | 46.61 |
| ATOM | 2928 | N   | ASP | A | 373 | 0.225  | 40.488 | 73.993 | 1.00 | 22.30 |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 2929 | CA  | ASP | A | 373 | 0.645  | 41.274 | 72.826 | 1.00 | 21.27 |
| ATOM | 2930 | C   | ASP | A | 373 | 2.131  | 41.004 | 72.577 | 1.00 | 25.86 |
| ATOM | 2931 | O   | ASP | A | 373 | 2.974  | 41.293 | 73.442 | 1.00 | 23.22 |
| ATOM | 2932 | CB  | ASP | A | 373 | 0.424  | 42.793 | 73.054 | 1.00 | 22.31 |
| ATOM | 2933 | CG  | ASP | A | 373 | 0.891  | 43.654 | 71.883 | 1.00 | 29.73 |
| ATOM | 2934 | OD1 | ASP | A | 373 | 1.515  | 43.194 | 70.941 | 1.00 | 31.76 |
| ATOM | 2935 | OD2 | ASP | A | 373 | 0.555  | 44.930 | 71.969 | 1.00 | 27.86 |
| ATOM | 2936 | N   | PRO | A | 374 | 2.484  | 40.463 | 71.409 | 1.00 | 22.50 |
| ATOM | 2937 | CA  | PRO | A | 374 | 3.889  | 40.171 | 71.166 | 1.00 | 23.16 |
| ATOM | 2938 | C   | PRO | A | 374 | 4.850  | 41.301 | 71.504 | 1.00 | 24.89 |
| ATOM | 2939 | O   | PRO | A | 374 | 5.888  | 41.089 | 72.161 | 1.00 | 21.00 |
| ATOM | 2940 | CB  | PRO | A | 374 | 3.997  | 39.698 | 69.728 | 1.00 | 23.24 |
| ATOM | 2941 | CG  | PRO | A | 374 | 2.640  | 39.097 | 69.454 | 1.00 | 24.05 |
| ATOM | 2942 | CD  | PRO | A | 374 | 1.667  | 39.848 | 70.346 | 1.00 | 21.54 |
| ATOM | 2943 | N   | ASP | A | 375 | 4.497  | 42.498 | 71.044 | 1.00 | 20.29 |
| ATOM | 2944 | CA  | ASP | A | 375 | 5.313  | 43.679 | 71.309 | 1.00 | 19.41 |
| ATOM | 2945 | C   | ASP | A | 375 | 5.632  | 43.849 | 72.789 | 1.00 | 22.07 |
| ATOM | 2946 | O   | ASP | A | 375 | 6.619  | 44.453 | 73.160 | 1.00 | 22.53 |
| ATOM | 2947 | CB  | ASP | A | 375 | 4.539  | 44.916 | 70.867 | 1.00 | 18.53 |
| ATOM | 2948 | CG  | ASP | A | 375 | 4.597  | 45.029 | 69.394 | 1.00 | 26.47 |
| ATOM | 2949 | OD1 | ASP | A | 375 | 5.523  | 44.560 | 68.735 | 1.00 | 24.70 |
| ATOM | 2950 | OD2 | ASP | A | 375 | 3.591  | 45.714 | 68.900 | 1.00 | 27.57 |
| ATOM | 2951 | N   | VAL | A | 376 | 4.752  | 43.349 | 73.624 | 1.00 | 18.89 |
| ATOM | 2952 | CA  | VAL | A | 376 | 4.911  | 43.461 | 75.053 | 1.00 | 20.94 |
| ATOM | 2953 | C   | VAL | A | 376 | 5.827  | 42.362 | 75.581 | 1.00 | 23.60 |
| ATOM | 2954 | O   | VAL | A | 376 | 6.514  | 42.551 | 76.560 | 1.00 | 22.26 |
| ATOM | 2955 | CB  | VAL | A | 376 | 3.530  | 43.386 | 75.725 | 1.00 | 24.27 |
| ATOM | 2956 | CG1 | VAL | A | 376 | 3.614  | 42.799 | 77.113 | 1.00 | 24.15 |
| ATOM | 2957 | CG2 | VAL | A | 376 | 2.846  | 44.741 | 75.763 | 1.00 | 21.88 |
| ATOM | 2958 | N   | ALA | A | 377 | 5.841  | 41.202 | 74.924 | 1.00 | 20.52 |
| ATOM | 2959 | CA  | ALA | A | 377 | 6.671  | 40.081 | 75.380 | 1.00 | 19.34 |
| ATOM | 2960 | C   | ALA | A | 377 | 8.119  | 40.144 | 74.936 | 1.00 | 21.06 |
| ATOM | 2961 | O   | ALA | A | 377 | 8.995  | 39.531 | 75.509 | 1.00 | 20.54 |
| ATOM | 2962 | CB  | ALA | A | 377 | 6.077  | 38.746 | 74.916 | 1.00 | 19.29 |
| ATOM | 2963 | N   | TYR | A | 378 | 8.349  | 40.881 | 73.894 | 1.00 | 18.62 |
| ATOM | 2964 | CA  | TYR | A | 378 | 9.653  | 41.015 | 73.291 | 1.00 | 18.37 |
| ATOM | 2965 | C   | TYR | A | 378 | 10.771 | 41.278 | 74.262 | 1.00 | 23.29 |
| ATOM | 2966 | O   | TYR | A | 378 | 10.680 | 42.178 | 75.069 | 1.00 | 21.02 |
| ATOM | 2967 | CB  | TYR | A | 378 | 9.627  | 42.149 | 72.292 | 1.00 | 18.13 |
| ATOM | 2968 | CG  | TYR | A | 378 | 10.914 | 42.258 | 71.523 | 1.00 | 18.41 |
| ATOM | 2969 | CD1 | TYR | A | 378 | 11.271 | 41.249 | 70.629 | 1.00 | 18.40 |
| ATOM | 2970 | CD2 | TYR | A | 378 | 11.752 | 43.361 | 71.682 | 1.00 | 17.09 |
| ATOM | 2971 | CE1 | TYR | A | 378 | 12.447 | 41.326 | 69.885 | 1.00 | 16.77 |
| ATOM | 2972 | CE2 | TYR | A | 378 | 12.933 | 43.450 | 70.942 | 1.00 | 17.00 |
| ATOM | 2973 | CZ  | TYR | A | 378 | 13.280 | 42.433 | 70.048 | 1.00 | 19.25 |
| ATOM | 2974 | OH  | TYR | A | 378 | 14.460 | 42.510 | 69.311 | 1.00 | 20.79 |
| ATOM | 2975 | N   | SER | A | 379 | 11.853 | 40.510 | 74.137 | 1.00 | 17.96 |
| ATOM | 2976 | CA  | SER | A | 379 | 13.014 | 40.665 | 74.999 | 1.00 | 16.74 |
| ATOM | 2977 | C   | SER | A | 379 | 14.186 | 39.980 | 74.376 | 1.00 | 18.88 |
| ATOM | 2978 | O   | SER | A | 379 | 14.077 | 39.440 | 73.300 | 1.00 | 17.88 |
| ATOM | 2979 | CB  | SER | A | 379 | 12.818 | 40.037 | 76.382 | 1.00 | 18.10 |
| ATOM | 2980 | OG  | SER | A | 379 | 12.971 | 38.616 | 76.326 | 1.00 | 17.76 |
| ATOM | 2981 | N   | SER | A | 380 | 15.304 | 39.989 | 75.093 | 1.00 | 17.79 |
| ATOM | 2982 | CA  | SER | A | 380 | 16.566 | 39.332 | 74.679 | 1.00 | 17.84 |
| ATOM | 2983 | C   | SER | A | 380 | 16.535 | 37.832 | 74.918 | 1.00 | 19.09 |
| ATOM | 2984 | O   | SER | A | 380 | 17.373 | 37.094 | 74.438 | 1.00 | 19.70 |
| ATOM | 2985 | CB  | SER | A | 380 | 17.713 | 39.827 | 75.547 | 1.00 | 22.61 |
| ATOM | 2986 | OG  | SER | A | 380 | 18.062 | 41.128 | 75.175 | 1.00 | 37.65 |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 2987 | N   | VAL | A | 381 | 15.584 | 37.373 | 75.701 | 1.00 | 15.92 |
| ATOM | 2988 | CA  | VAL | A | 381 | 15.506 | 35.970 | 75.994 | 1.00 | 13.28 |
| ATOM | 2989 | C   | VAL | A | 381 | 15.563 | 35.076 | 74.757 | 1.00 | 17.08 |
| ATOM | 2990 | O   | VAL | A | 381 | 16.405 | 34.186 | 74.689 | 1.00 | 16.24 |
| ATOM | 2991 | CB  | VAL | A | 381 | 14.307 | 35.616 | 76.897 | 1.00 | 14.10 |
| ATOM | 2992 | CG1 | VAL | A | 381 | 14.159 | 34.101 | 77.046 | 1.00 | 12.50 |
| ATOM | 2993 | CG2 | VAL | A | 381 | 14.465 | 36.274 | 78.251 | 1.00 | 13.34 |
| ATOM | 2994 | N   | PRO | A | 382 | 14.662 | 35.231 | 73.784 | 1.00 | 14.08 |
| ATOM | 2995 | CA  | PRO | A | 382 | 14.745 | 34.310 | 72.672 | 1.00 | 14.26 |
| ATOM | 2996 | C   | PRO | A | 382 | 16.092 | 34.383 | 71.956 | 1.00 | 19.53 |
| ATOM | 2997 | O   | PRO | A | 382 | 16.583 | 33.396 | 71.390 | 1.00 | 17.52 |
| ATOM | 2998 | CB  | PRO | A | 382 | 13.556 | 34.579 | 71.743 | 1.00 | 13.55 |
| ATOM | 2999 | CG  | PRO | A | 382 | 13.121 | 35.968 | 72.129 | 1.00 | 16.51 |
| ATOM | 3000 | CD  | PRO | A | 382 | 13.525 | 36.140 | 73.581 | 1.00 | 13.04 |
| ATOM | 3001 | N   | TYR | A | 383 | 16.712 | 35.556 | 71.988 | 1.00 | 14.90 |
| ATOM | 3002 | CA  | TYR | A | 383 | 17.995 | 35.727 | 71.326 | 1.00 | 15.56 |
| ATOM | 3003 | C   | TYR | A | 383 | 19.142 | 35.019 | 72.036 | 1.00 | 19.49 |
| ATOM | 3004 | O   | TYR | A | 383 | 19.942 | 34.276 | 71.454 | 1.00 | 18.21 |
| ATOM | 3005 | CB  | TYR | A | 383 | 18.371 | 37.226 | 71.280 | 1.00 | 16.26 |
| ATOM | 3006 | CG  | TYR | A | 383 | 17.518 | 38.078 | 70.360 | 1.00 | 17.31 |
| ATOM | 3007 | CD1 | TYR | A | 383 | 16.257 | 38.519 | 70.768 | 1.00 | 17.98 |
| ATOM | 3008 | CD2 | TYR | A | 383 | 17.984 | 38.490 | 69.106 | 1.00 | 15.67 |
| ATOM | 3009 | CE1 | TYR | A | 383 | 15.462 | 39.310 | 69.936 | 1.00 | 17.12 |
| ATOM | 3010 | CE2 | TYR | A | 383 | 17.202 | 39.274 | 68.259 | 1.00 | 17.10 |
| ATOM | 3011 | CZ  | TYR | A | 383 | 15.940 | 39.688 | 68.686 | 1.00 | 22.02 |
| ATOM | 3012 | OH  | TYR | A | 383 | 15.158 | 40.465 | 67.893 | 1.00 | 18.91 |
| ATOM | 3013 | N   | GLU | A | 384 | 19.227 | 35.308 | 73.306 | 1.00 | 14.23 |
| ATOM | 3014 | CA  | GLU | A | 384 | 20.301 | 34.842 | 74.136 | 1.00 | 12.36 |
| ATOM | 3015 | C   | GLU | A | 384 | 20.128 | 33.494 | 74.752 | 1.00 | 17.78 |
| ATOM | 3016 | O   | GLU | A | 384 | 21.096 | 32.756 | 74.866 | 1.00 | 14.92 |
| ATOM | 3017 | CB  | GLU | A | 384 | 20.707 | 35.952 | 75.093 | 1.00 | 12.48 |
| ATOM | 3018 | CG  | GLU | A | 384 | 21.058 | 37.217 | 74.275 | 1.00 | 15.08 |
| ATOM | 3019 | CD  | GLU | A | 384 | 22.403 | 37.098 | 73.589 | 1.00 | 31.19 |
| ATOM | 3020 | OE1 | GLU | A | 384 | 23.132 | 36.113 | 73.647 | 1.00 | 22.19 |
| ATOM | 3021 | OE2 | GLU | A | 384 | 22.720 | 38.171 | 72.935 | 1.00 | 23.77 |
| ATOM | 3022 | N   | LYS | A | 385 | 18.897 | 33.118 | 75.133 | 1.00 | 16.58 |
| ATOM | 3023 | CA  | LYS | A | 385 | 18.771 | 31.759 | 75.664 | 1.00 | 16.36 |
| ATOM | 3024 | C   | LYS | A | 385 | 18.891 | 30.809 | 74.458 | 1.00 | 16.81 |
| ATOM | 3025 | O   | LYS | A | 385 | 19.449 | 29.705 | 74.540 | 1.00 | 15.97 |
| ATOM | 3026 | CB  | LYS | A | 385 | 17.514 | 31.508 | 76.512 | 1.00 | 14.73 |
| ATOM | 3027 | CG  | LYS | A | 385 | 17.557 | 30.142 | 77.175 | 1.00 | 12.89 |
| ATOM | 3028 | CD  | LYS | A | 385 | 16.295 | 29.802 | 77.949 | 1.00 | 25.17 |
| ATOM | 3029 | CE  | LYS | A | 385 | 16.211 | 30.454 | 79.301 | 1.00 | 20.12 |
| ATOM | 3030 | NZ  | LYS | A | 385 | 15.202 | 29.829 | 80.175 | 1.00 | 16.04 |
| ATOM | 3031 | N   | GLY | A | 386 | 18.374 | 31.286 | 73.316 | 1.00 | 12.80 |
| ATOM | 3032 | CA  | GLY | A | 386 | 18.421 | 30.480 | 72.112 | 1.00 | 11.62 |
| ATOM | 3033 | C   | GLY | A | 386 | 19.866 | 30.250 | 71.689 | 1.00 | 17.22 |
| ATOM | 3034 | O   | GLY | A | 386 | 20.289 | 29.130 | 71.430 | 1.00 | 17.34 |
| ATOM | 3035 | N   | PHE | A | 387 | 20.623 | 31.333 | 71.580 | 1.00 | 14.79 |
| ATOM | 3036 | CA  | PHE | A | 387 | 22.018 | 31.218 | 71.214 | 1.00 | 15.40 |
| ATOM | 3037 | C   | PHE | A | 387 | 22.766 | 30.353 | 72.238 | 1.00 | 19.58 |
| ATOM | 3038 | O   | PHE | A | 387 | 23.557 | 29.502 | 71.884 | 1.00 | 19.03 |
| ATOM | 3039 | CB  | PHE | A | 387 | 22.686 | 32.579 | 71.045 | 1.00 | 14.79 |
| ATOM | 3040 | CG  | PHE | A | 387 | 24.167 | 32.431 | 70.988 | 1.00 | 13.37 |
| ATOM | 3041 | CD1 | PHE | A | 387 | 24.895 | 32.181 | 69.815 | 1.00 | 14.32 |
| ATOM | 3042 | CD2 | PHE | A | 387 | 24.842 | 32.519 | 72.202 | 1.00 | 14.90 |
| ATOM | 3043 | CE1 | PHE | A | 387 | 26.287 | 32.043 | 69.857 | 1.00 | 12.12 |
| ATOM | 3044 | CE2 | PHE | A | 387 | 26.233 | 32.407 | 72.259 | 1.00 | 15.96 |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 3045 | CZ  | PHE | A | 387 | 26.954 | 32.148 | 71.086 | 1.00 | 14.94 |
| ATOM | 3046 | N   | ALA | A | 388 | 22.487 | 30.533 | 73.522 | 1.00 | 16.65 |
| ATOM | 3047 | CA  | ALA | A | 388 | 23.138 | 29.706 | 74.541 | 1.00 | 17.04 |
| ATOM | 3048 | C   | ALA | A | 388 | 22.865 | 28.231 | 74.291 | 1.00 | 19.93 |
| ATOM | 3049 | O   | ALA | A | 388 | 23.775 | 27.412 | 74.356 | 1.00 | 20.75 |
| ATOM | 3050 | CB  | ALA | A | 388 | 22.644 | 30.086 | 75.936 | 1.00 | 17.04 |
| ATOM | 3051 | N   | LEU | A | 389 | 21.595 | 27.878 | 74.017 | 1.00 | 13.52 |
| ATOM | 3052 | CA  | LEU | A | 389 | 21.270 | 26.481 | 73.746 | 1.00 | 12.75 |
| ATOM | 3053 | C   | LEU | A | 389 | 22.142 | 25.954 | 72.616 | 1.00 | 16.14 |
| ATOM | 3054 | O   | LEU | A | 389 | 22.804 | 24.921 | 72.761 | 1.00 | 15.90 |
| ATOM | 3055 | CB  | LEU | A | 389 | 19.792 | 26.354 | 73.374 | 1.00 | 11.62 |
| ATOM | 3056 | CG  | LEU | A | 389 | 19.364 | 24.983 | 72.909 | 1.00 | 15.19 |
| ATOM | 3057 | CD1 | LEU | A | 389 | 19.839 | 23.930 | 73.914 | 1.00 | 16.82 |
| ATOM | 3058 | CD2 | LEU | A | 389 | 17.839 | 24.969 | 72.839 | 1.00 | 15.73 |
| ATOM | 3059 | N   | LEU | A | 390 | 22.149 | 26.690 | 71.503 | 1.00 | 12.97 |
| ATOM | 3060 | CA  | LEU | A | 390 | 22.939 | 26.331 | 70.348 | 1.00 | 13.79 |
| ATOM | 3061 | C   | LEU | A | 390 | 24.426 | 26.247 | 70.629 | 1.00 | 23.60 |
| ATOM | 3062 | O   | LEU | A | 390 | 25.099 | 25.328 | 70.136 | 1.00 | 22.90 |
| ATOM | 3063 | CB  | LEU | A | 390 | 22.718 | 27.238 | 69.141 | 1.00 | 12.43 |
| ATOM | 3064 | CG  | LEU | A | 390 | 21.238 | 27.308 | 68.754 | 1.00 | 16.53 |
| ATOM | 3065 | CD1 | LEU | A | 390 | 21.063 | 28.259 | 67.570 | 1.00 | 17.80 |
| ATOM | 3066 | CD2 | LEU | A | 390 | 20.706 | 25.916 | 68.416 | 1.00 | 19.39 |
| ATOM | 3067 | N   | PHE | A | 391 | 24.950 | 27.195 | 71.406 | 1.00 | 17.01 |
| ATOM | 3068 | CA  | PHE | A | 391 | 26.383 | 27.213 | 71.707 | 1.00 | 13.81 |
| ATOM | 3069 | C   | PHE | A | 391 | 26.767 | 25.994 | 72.507 | 1.00 | 18.97 |
| ATOM | 3070 | O   | PHE | A | 391 | 27.788 | 25.335 | 72.292 | 1.00 | 17.39 |
| ATOM | 3071 | CB  | PHE | A | 391 | 26.716 | 28.464 | 72.505 | 1.00 | 16.57 |
| ATOM | 3072 | CG  | PHE | A | 391 | 28.178 | 28.832 | 72.483 | 1.00 | 20.15 |
| ATOM | 3073 | CD1 | PHE | A | 391 | 28.900 | 28.717 | 71.295 | 1.00 | 23.44 |
| ATOM | 3074 | CD2 | PHE | A | 391 | 28.810 | 29.322 | 73.629 | 1.00 | 17.67 |
| ATOM | 3075 | CE1 | PHE | A | 391 | 30.242 | 29.081 | 71.247 | 1.00 | 25.42 |
| ATOM | 3076 | CE2 | PHE | A | 391 | 30.161 | 29.679 | 73.600 | 1.00 | 21.60 |
| ATOM | 3077 | CZ  | PHE | A | 391 | 30.872 | 29.552 | 72.404 | 1.00 | 21.74 |
| ATOM | 3078 | N   | TYR | A | 392 | 25.899 | 25.688 | 73.453 | 1.00 | 16.76 |
| ATOM | 3079 | CA  | TYR | A | 392 | 26.093 | 24.528 | 74.314 | 1.00 | 14.53 |
| ATOM | 3080 | C   | TYR | A | 392 | 26.030 | 23.258 | 73.477 | 1.00 | 20.85 |
| ATOM | 3081 | O   | TYR | A | 392 | 26.888 | 22.387 | 73.570 | 1.00 | 21.28 |
| ATOM | 3082 | CB  | TYR | A | 392 | 25.011 | 24.548 | 75.389 | 1.00 | 11.64 |
| ATOM | 3083 | CG  | TYR | A | 392 | 24.758 | 23.236 | 76.085 | 1.00 | 15.88 |
| ATOM | 3084 | CD1 | TYR | A | 392 | 25.675 | 22.664 | 76.969 | 1.00 | 18.73 |
| ATOM | 3085 | CD2 | TYR | A | 392 | 23.536 | 22.598 | 75.901 | 1.00 | 17.10 |
| ATOM | 3086 | CE1 | TYR | A | 392 | 25.398 | 21.453 | 77.611 | 1.00 | 22.29 |
| ATOM | 3087 | CE2 | TYR | A | 392 |        |        |        |      |       |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 3103 | CG  | GLU | A | 394 | 29.691 | 24.466 | 68.704 | 1.00 | 21.87 |
| ATOM | 3104 | CD  | GLU | A | 394 | 30.088 | 25.892 | 68.499 | 1.00 | 35.26 |
| ATOM | 3105 | OE1 | GLU | A | 394 | 29.443 | 26.672 | 67.835 | 1.00 | 37.15 |
| ATOM | 3106 | OE2 | GLU | A | 394 | 31.185 | 26.212 | 69.125 | 1.00 | 23.86 |
| ATOM | 3107 | N   | GLN | A | 395 | 29.226 | 22.758 | 71.574 | 1.00 | 20.49 |
| ATOM | 3108 | CA  | GLN | A | 395 | 30.303 | 22.250 | 72.400 | 1.00 | 20.42 |
| ATOM | 3109 | C   | GLN | A | 395 | 30.092 | 20.769 | 72.720 | 1.00 | 25.74 |
| ATOM | 3110 | O   | GLN | A | 395 | 31.016 | 19.972 | 72.734 | 1.00 | 29.45 |
| ATOM | 3111 | CB  | GLN | A | 395 | 30.474 | 23.105 | 73.709 | 1.00 | 20.72 |
| ATOM | 3112 | CG  | GLN | A | 395 | 31.074 | 24.483 | 73.365 | 1.00 | 15.91 |
| ATOM | 3113 | CD  | GLN | A | 395 | 31.156 | 25.473 | 74.518 | 1.00 | 23.39 |
| ATOM | 3114 | OE1 | GLN | A | 395 | 30.799 | 25.196 | 75.685 | 1.00 | 18.07 |
| ATOM | 3115 | NE2 | GLN | A | 395 | 31.625 | 26.663 | 74.177 | 1.00 | 21.74 |
| ATOM | 3116 | N   | LEU | A | 396 | 28.851 | 20.406 | 72.981 | 1.00 | 21.83 |
| ATOM | 3117 | CA  | LEU | A | 396 | 28.497 | 19.046 | 73.343 | 1.00 | 20.76 |
| ATOM | 3118 | C   | LEU | A | 396 | 28.638 | 18.071 | 72.176 | 1.00 | 23.05 |
| ATOM | 3119 | O   | LEU | A | 396 | 29.032 | 16.938 | 72.337 | 1.00 | 23.88 |
| ATOM | 3120 | CB  | LEU | A | 396 | 27.054 | 19.104 | 73.857 | 1.00 | 20.00 |
| ATOM | 3121 | CG  | LEU | A | 396 | 26.555 | 17.836 | 74.446 | 1.00 | 25.23 |
| ATOM | 3122 | CD1 | LEU | A | 396 | 27.296 | 17.572 | 75.738 | 1.00 | 28.56 |
| ATOM | 3123 | CD2 | LEU | A | 396 | 25.087 | 18.002 | 74.744 | 1.00 | 24.07 |
| ATOM | 3124 | N   | LEU | A | 397 | 28.328 | 18.524 | 70.994 | 1.00 | 18.54 |
| ATOM | 3125 | CA  | LEU | A | 397 | 28.351 | 17.694 | 69.808 | 1.00 | 19.54 |
| ATOM | 3126 | C   | LEU | A | 397 | 29.641 | 17.641 | 69.009 | 1.00 | 27.29 |
| ATOM | 3127 | O   | LEU | A | 397 | 29.710 | 16.985 | 67.968 | 1.00 | 28.65 |
| ATOM | 3128 | CB  | LEU | A | 397 | 27.143 | 18.043 | 68.891 | 1.00 | 17.91 |
| ATOM | 3129 | CG  | LEU | A | 397 | 25.798 | 17.909 | 69.619 | 1.00 | 20.05 |
| ATOM | 3130 | CD1 | LEU | A | 397 | 24.671 | 18.520 | 68.789 | 1.00 | 18.08 |
| ATOM | 3131 | CD2 | LEU | A | 397 | 25.520 | 16.443 | 69.920 | 1.00 | 21.42 |
| ATOM | 3132 | N   | GLY | A | 398 | 30.685 | 18.313 | 69.425 | 1.00 | 25.76 |
| ATOM | 3133 | CA  | GLY | A | 398 | 31.896 | 18.173 | 68.621 | 1.00 | 27.87 |
| ATOM | 3134 | C   | GLY | A | 398 | 32.558 | 19.413 | 68.060 | 1.00 | 29.85 |
| ATOM | 3135 | O   | GLY | A | 398 | 33.621 | 19.303 | 67.448 | 1.00 | 28.10 |
| ATOM | 3136 | N   | GLY | A | 399 | 31.964 | 20.593 | 68.243 | 1.00 | 24.15 |
| ATOM | 3137 | CA  | GLY | A | 399 | 32.594 | 21.787 | 67.719 | 1.00 | 21.84 |
| ATOM | 3138 | C   | GLY | A | 399 | 31.801 | 22.444 | 66.626 | 1.00 | 20.27 |
| ATOM | 3139 | O   | GLY | A | 399 | 30.877 | 21.901 | 66.046 | 1.00 | 22.03 |
| ATOM | 3140 | N   | PRO | A | 400 | 32.210 | 23.639 | 66.373 | 1.00 | 21.16 |
| ATOM | 3141 | CA  | PRO | A | 400 | 31.596 | 24.524 | 65.434 | 1.00 | 21.61 |
| ATOM | 3142 | C   | PRO | A | 400 | 31.451 | 23.932 | 64.094 | 1.00 | 28.95 |
| ATOM | 3143 | O   | PRO | A | 400 | 30.416 | 24.076 | 63.432 | 1.00 | 28.40 |
| ATOM | 3144 | CB  | PRO | A | 400 | 32.477 | 25.776 | 65.359 | 1.00 | 22.74 |
| ATOM | 3145 | CG  | PRO | A |     |        |        |        |      |       |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 3161 | CG1 | ILE | A | 402 | 31.728 | 17.840 | 64.129 | 1.00 | 25.46 |
| ATOM | 3162 | CG2 | ILE | A | 402 | 29.257 | 18.044 | 64.720 | 1.00 | 31.45 |
| ATOM | 3163 | CD1 | ILE | A | 402 | 32.086 | 16.989 | 65.348 | 1.00 | 29.47 |
| ATOM | 3164 | N   | PHE | A | 403 | 28.806 | 21.270 | 64.247 | 1.00 | 25.40 |
| ATOM | 3165 | CA  | PHE | A | 403 | 27.539 | 21.974 | 64.418 | 1.00 | 23.64 |
| ATOM | 3166 | C   | PHE | A | 403 | 27.131 | 22.827 | 63.207 | 1.00 | 24.67 |
| ATOM | 3167 | O   | PHE | A | 403 | 25.940 | 22.935 | 62.860 | 1.00 | 23.76 |
| ATOM | 3168 | CB  | PHE | A | 403 | 27.484 | 22.767 | 65.750 | 1.00 | 23.99 |
| ATOM | 3169 | CG  | PHE | A | 403 | 26.066 | 22.896 | 66.252 | 1.00 | 23.55 |
| ATOM | 3170 | CD1 | PHE | A | 403 | 25.432 | 21.835 | 66.909 | 1.00 | 25.66 |
| ATOM | 3171 | CD2 | PHE | A | 403 | 25.369 | 24.089 | 66.045 | 1.00 | 23.45 |
| ATOM | 3172 | CE1 | PHE | A | 403 | 24.119 | 21.961 | 67.368 | 1.00 | 26.71 |
| ATOM | 3173 | CE2 | PHE | A | 403 | 24.065 | 24.245 | 66.507 | 1.00 | 24.58 |
| ATOM | 3174 | CZ  | PHE | A | 403 | 23.454 | 23.174 | 67.161 | 1.00 | 24.36 |
| ATOM | 3175 | N   | LEU | A | 404 | 28.103 | 23.454 | 62.565 | 1.00 | 18.37 |
| ATOM | 3176 | CA  | LEU | A | 404 | 27.752 | 24.224 | 61.396 | 1.00 | 19.70 |
| ATOM | 3177 | C   | LEU | A | 404 | 27.161 | 23.330 | 60.312 | 1.00 | 23.87 |
| ATOM | 3178 | O   | LEU | A | 404 | 26.262 | 23.753 | 59.594 | 1.00 | 22.72 |
| ATOM | 3179 | CB  | LEU | A | 404 | 28.867 | 25.117 | 60.847 | 1.00 | 20.74 |
| ATOM | 3180 | CG  | LEU | A | 404 | 29.026 | 26.425 | 61.635 | 1.00 | 24.87 |
| ATOM | 3181 | CD1 | LEU | A | 404 | 30.384 | 27.056 | 61.345 | 1.00 | 26.17 |
| ATOM | 3182 | CD2 | LEU | A | 404 | 27.944 | 27.424 | 61.266 | 1.00 | 19.99 |
| ATOM | 3183 | N   | GLY | A | 405 | 27.662 | 22.078 | 60.205 | 1.00 | 20.85 |
| ATOM | 3184 | CA  | GLY | A | 405 | 27.173 | 21.098 | 59.225 | 1.00 | 16.93 |
| ATOM | 3185 | C   | GLY | A | 405 | 25.687 | 20.844 | 59.464 | 1.00 | 20.17 |
| ATOM | 3186 | O   | GLY | A | 405 | 24.872 | 20.712 | 58.556 | 1.00 | 19.11 |
| ATOM | 3187 | N   | PHE | A | 406 | 25.346 | 20.814 | 60.739 | 1.00 | 18.34 |
| ATOM | 3188 | CA  | PHE | A | 406 | 23.968 | 20.629 | 61.142 | 1.00 | 19.38 |
| ATOM | 3189 | C   | PHE | A | 406 | 23.149 | 21.854 | 60.701 | 1.00 | 24.71 |
| ATOM | 3190 | O   | PHE | A | 406 | 22.127 | 21.736 | 60.016 | 1.00 | 24.92 |
| ATOM | 3191 | CB  | PHE | A | 406 | 23.811 | 20.239 | 62.626 | 1.00 | 17.08 |
| ATOM | 3192 | CG  | PHE | A | 406 | 22.440 | 20.588 | 63.100 | 1.00 | 17.29 |
| ATOM | 3193 | CD1 | PHE | A | 406 | 21.348 | 19.779 | 62.795 | 1.00 | 18.79 |
| ATOM | 3194 | CD2 | PHE | A | 406 | 22.229 | 21.756 | 63.819 | 1.00 | 22.17 |
| ATOM | 3195 | CE1 | PHE | A | 406 | 20.066 | 20.089 | 63.242 | 1.00 | 21.72 |
| ATOM | 3196 | CE2 | PHE | A | 406 | 20.949 | 22.108 | 64.245 | 1.00 | 25.55 |
| ATOM | 3197 | CZ  | PHE | A | 406 | 19.872 | 21.266 | 63.966 | 1.00 | 23.17 |
| ATOM | 3198 | N   | LEU | A | 407 | 23.637 | 23.049 | 61.028 | 1.00 | 23.64 |
| ATOM | 3199 | CA  | LEU | A | 407 | 22.944 | 24.287 | 60.642 | 1.00 | 24.87 |
| ATOM | 3200 | C   | LEU | A | 407 | 22.597 | 24.312 | 59.161 | 1.00 | 22.41 |
| ATOM | 3201 | O   | LEU | A | 407 | 21.479 | 24.620 | 58.769 | 1.00 | 20.72 |
| ATOM | 3202 | CB  | LEU | A | 407 | 23.791 | 25.560 | 60.959 | 1.00 | 27.52 |
| ATOM | 3203 | CG  | LEU | A | 407 | 23.074 | 26.747 | 61.652 | 1.00 | 34.83 |
| ATOM | 3204 | CD1 | LEU | A | 407 | 24.068 | 27.866 | 61.821 | 1.00 | 38.37 |
| ATOM | 3205 | CD2 | LEU | A | 407 | 21.906 | 27.303 | 60.863 | 1.00 | 36.77 |
| ATOM | 3206 | N   | LYS | A | 408 | 23.587 | 24.048 | 58.315 | 1.00 | 22.80 |
| ATOM | 3207 | CA  | LYS | A | 408 | 23.364 | 24.064 | 56.871 | 1.00 | 23.13 |
| ATOM | 3208 | C   | LYS | A | 408 | 22.352 | 22.998 | 56.426 | 1.00 | 22.11 |
| ATOM | 3209 | O   | LYS | A | 408 | 21.517 | 23.175 | 55.536 | 1.00 | 20.19 |
| ATOM | 3210 | CB  | LYS | A | 408 | 24.650 | 23.961 | 56.082 | 1.00 | 25.07 |
| ATOM | 3211 | CG  | LYS | A | 408 | 24.372 | 24.064 | 54.599 | 1.00 | 31.85 |
| ATOM | 3212 | CD  | LYS | A | 408 | 25.620 | 24.004 | 53.740 | 1.00 | 30.52 |
| ATOM | 3213 | CE  | LYS | A | 408 | 26.712 | 24.948 | 54.189 | 1.00 | 44.55 |
| ATOM | 3214 | NZ  | LYS | A | 408 | 27.738 | 25.166 | 53.153 | 1.00 | 52.58 |
| ATOM | 3215 | N   | ALA | A | 409 | 22.423 | 21.861 | 57.066 | 1.00 | 20.83 |
| ATOM | 3216 | CA  | ALA | A | 409 | 21.481 | 20.812 | 56.728 | 1.00 | 23.36 |
| ATOM | 3217 | C   | ALA | A | 409 | 20.047 | 21.215 | 57.138 | 1.00 | 25.95 |
| ATOM | 3218 | O   | ALA | A | 409 | 19.062 | 20.940 | 56.447 | 1.00 | 23.39 |



|      |      |     |     |   |     |        |        |        |      |        |
|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
| ATOM | 3219 | CB  | ALA | A | 409 | 21.892 | 19.518 | 57.422 | 1.00 | 24.61  |
| ATOM | 3220 | N   | TYR | A | 410 | 19.971 | 21.870 | 58.295 | 1.00 | 18.99  |
| ATOM | 3221 | CA  | TYR | A | 410 | 18.742 | 22.373 | 58.878 | 1.00 | 17.32  |
| ATOM | 3222 | C   | TYR | A | 410 | 18.076 | 23.378 | 57.950 | 1.00 | 20.68  |
| ATOM | 3223 | O   | TYR | A | 410 | 16.882 | 23.297 | 57.646 | 1.00 | 20.76  |
| ATOM | 3224 | CB  | TYR | A | 410 | 19.046 | 23.007 | 60.248 | 1.00 | 18.05  |
| ATOM | 3225 | CG  | TYR | A | 410 | 17.953 | 23.881 | 60.833 | 1.00 | 21.53  |
| ATOM | 3226 | CD1 | TYR | A | 410 | 16.772 | 23.334 | 61.341 | 1.00 | 22.90  |
| ATOM | 3227 | CD2 | TYR | A | 410 | 18.137 | 25.262 | 60.913 | 1.00 | 24.29  |
| ATOM | 3228 | CE1 | TYR | A | 410 | 15.778 | 24.149 | 61.887 | 1.00 | 18.00  |
| ATOM | 3229 | CE2 | TYR | A | 410 | 17.168 | 26.093 | 61.469 | 1.00 | 24.98  |
| ATOM | 3230 | CZ  | TYR | A | 410 | 15.993 | 25.526 | 61.954 | 1.00 | 20.26  |
| ATOM | 3231 | OH  | TYR | A | 410 | 15.056 | 26.328 | 62.527 | 1.00 | 21.69  |
| ATOM | 3232 | N   | VAL | A | 411 | 18.869 | 24.318 | 57.491 | 1.00 | 15.71  |
| ATOM | 3233 | CA  | VAL | A | 411 | 18.383 | 25.335 | 56.612 | 1.00 | 17.92  |
| ATOM | 3234 | C   | VAL | A | 411 | 17.783 | 24.734 | 55.369 | 1.00 | 23.98  |
| ATOM | 3235 | O   | VAL | A | 411 | 16.701 | 25.099 | 54.974 | 1.00 | 24.28  |
| ATOM | 3236 | CB  | VAL | A | 411 | 19.511 | 26.312 | 56.254 | 1.00 | 23.58  |
| ATOM | 3237 | CG1 | VAL | A | 411 | 19.094 | 27.279 | 55.139 | 1.00 | 22.54  |
| ATOM | 3238 | CG2 | VAL | A | 411 | 19.940 | 27.085 | 57.505 | 1.00 | 24.67  |
| ATOM | 3239 | N   | GLU | A | 412 | 18.543 | 23.824 | 54.750 | 1.00 | 25.06  |
| ATOM | 3240 | CA  | GLU | A | 412 | 18.177 | 23.124 | 53.539 | 1.00 | 22.96  |
| ATOM | 3241 | C   | GLU | A | 412 | 16.919 | 22.318 | 53.715 | 1.00 | 23.85  |
| ATOM | 3242 | O   | GLU | A | 412 | 16.023 | 22.366 | 52.883 | 1.00 | 22.54  |
| ATOM | 3243 | CB  | GLU | A | 412 | 19.302 | 22.173 | 53.210 | 1.00 | 26.35  |
| ATOM | 3244 | CG  | GLU | A | 412 | 19.444 | 21.914 | 51.707 | 1.00 | 49.27  |
| ATOM | 3245 | CD  | GLU | A | 412 | 20.800 | 21.342 | 51.380 | 1.00 | 100.00 |
| ATOM | 3246 | OE1 | GLU | A | 412 | 21.851 | 21.791 | 51.838 | 1.00 | 100.00 |
| ATOM | 3247 | OE2 | GLU | A | 412 | 20.727 | 20.308 | 50.566 | 1.00 | 100.00 |
| ATOM | 3248 | N   | LYS | A | 413 | 16.854 | 21.581 | 54.824 | 1.00 | 17.32  |
| ATOM | 3249 | CA  | LYS | A | 413 | 15.695 | 20.782 | 55.075 | 1.00 | 14.83  |
| ATOM | 3250 | C   | LYS | A | 413 | 14.415 | 21.569 | 55.203 | 1.00 | 20.01  |
| ATOM | 3251 | O   | LYS | A | 413 | 13.385 | 21.115 | 54.733 | 1.00 | 20.56  |
| ATOM | 3252 | CB  | LYS | A | 413 | 15.874 | 19.925 | 56.283 | 1.00 | 15.20  |
| ATOM | 3253 | CG  | LYS | A | 413 | 14.541 | 19.417 | 56.795 | 1.00 | 30.99  |
| ATOM | 3254 | CD  | LYS | A | 413 | 14.126 | 18.085 | 56.202 | 1.00 | 36.92  |
| ATOM | 3255 | CE  | LYS | A | 413 | 13.676 | 17.091 | 57.267 | 1.00 | 49.02  |
| ATOM | 3256 | NZ  | LYS | A | 413 | 13.031 | 15.887 | 56.725 | 1.00 | 66.84  |
| ATOM | 3257 | N   | PHE | A | 414 | 14.473 | 22.748 | 55.835 | 1.00 | 16.13  |
| ATOM | 3258 | CA  | PHE | A | 414 | 13.293 | 23.542 | 56.088 | 1.00 | 13.37  |
| ATOM | 3259 | C   | PHE | A | 414 | 13.145 | 24.807 | 55.296 | 1.00 | 20.62  |
| ATOM | 3260 | O   | PHE | A | 414 | 12.255 | 25.621 | 55.547 | 1.00 | 19.74  |
| ATOM | 3261 | CB  | PHE | A |     |        |        |        |      |        |



|      |      |     |     |   |     |        |        |        |      |        |
|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
| ATOM | 3277 | O   | TYR | A | 416 | 8.306  | 27.333 | 52.923 | 1.00 | 20.11  |
| ATOM | 3278 | CB  | TYR | A | 416 | 10.325 | 27.563 | 51.033 | 1.00 | 24.28  |
| ATOM | 3279 | CG  | TYR | A | 416 | 11.505 | 27.894 | 50.178 | 1.00 | 24.78  |
| ATOM | 3280 | CD1 | TYR | A | 416 | 12.358 | 26.878 | 49.745 | 1.00 | 24.62  |
| ATOM | 3281 | CD2 | TYR | A | 416 | 11.790 | 29.217 | 49.839 | 1.00 | 24.25  |
| ATOM | 3282 | CE1 | TYR | A | 416 | 13.483 | 27.163 | 48.979 | 1.00 | 19.21  |
| ATOM | 3283 | CE2 | TYR | A | 416 | 12.906 | 29.515 | 49.059 | 1.00 | 25.80  |
| ATOM | 3284 | CZ  | TYR | A | 416 | 13.749 | 28.484 | 48.635 | 1.00 | 28.59  |
| ATOM | 3285 | OH  | TYR | A | 416 | 14.859 | 28.745 | 47.870 | 1.00 | 32.88  |
| ATOM | 3286 | N   | LYS | A | 417 | 9.799  | 26.749 | 54.541 | 1.00 | 15.88  |
| ATOM | 3287 | CA  | LYS | A | 417 | 8.806  | 26.181 | 55.428 | 1.00 | 14.99  |
| ATOM | 3288 | C   | LYS | A | 417 | 8.702  | 27.001 | 56.708 | 1.00 | 19.80  |
| ATOM | 3289 | O   | LYS | A | 417 | 9.552  | 27.832 | 56.976 | 1.00 | 17.04  |
| ATOM | 3290 | CB  | LYS | A | 417 | 9.182  | 24.754 | 55.774 | 1.00 | 17.07  |
| ATOM | 3291 | CG  | LYS | A | 417 | 8.902  | 23.837 | 54.568 | 1.00 | 42.14  |
| ATOM | 3292 | CD  | LYS | A | 417 | 9.705  | 22.537 | 54.512 | 1.00 | 70.23  |
| ATOM | 3293 | CE  | LYS | A | 417 | 9.893  | 22.020 | 53.080 | 1.00 | 98.46  |
| ATOM | 3294 | NZ  | LYS | A | 417 | 11.308 | 21.895 | 52.655 | 1.00 | 100.00 |
| ATOM | 3295 | N   | SER | A | 418 | 7.656  | 26.770 | 57.483 | 1.00 | 18.76  |
| ATOM | 3296 | CA  | SER | A | 418 | 7.453  | 27.431 | 58.777 | 1.00 | 18.23  |
| ATOM | 3297 | C   | SER | A | 418 | 7.414  | 26.261 | 59.746 | 1.00 | 19.84  |
| ATOM | 3298 | O   | SER | A | 418 | 6.668  | 25.314 | 59.510 | 1.00 | 21.54  |
| ATOM | 3299 | CB  | SER | A | 418 | 6.204  | 28.273 | 58.786 | 1.00 | 19.06  |
| ATOM | 3300 | OG  | SER | A | 418 | 6.323  | 29.170 | 57.698 | 1.00 | 21.69  |
| ATOM | 3301 | N   | ILE | A | 419 | 8.262  | 26.253 | 60.778 | 1.00 | 15.55  |
| ATOM | 3302 | CA  | ILE | A | 419 | 8.365  | 25.081 | 61.648 | 1.00 | 15.71  |
| ATOM | 3303 | C   | ILE | A | 419 | 8.280  | 25.384 | 63.110 | 1.00 | 19.68  |
| ATOM | 3304 | O   | ILE | A | 419 | 8.328  | 26.531 | 63.526 | 1.00 | 17.46  |
| ATOM | 3305 | CB  | ILE | A | 419 | 9.747  | 24.424 | 61.410 | 1.00 | 18.62  |
| ATOM | 3306 | CG1 | ILE | A | 419 | 10.831 | 25.461 | 61.722 | 1.00 | 19.15  |
| ATOM | 3307 | CG2 | ILE | A | 419 | 9.918  | 24.029 | 59.951 | 1.00 | 17.84  |
| ATOM | 3308 | CD1 | ILE | A | 419 | 12.228 | 24.868 | 61.646 | 1.00 | 20.96  |
| ATOM | 3309 | N   | THR | A | 420 | 8.174  | 24.318 | 63.898 | 1.00 | 16.98  |
| ATOM | 3310 | CA  | THR | A | 420 | 8.093  | 24.498 | 65.337 | 1.00 | 16.43  |
| ATOM | 3311 | C   | THR | A | 420 | 9.348  | 23.960 | 65.974 | 1.00 | 21.83  |
| ATOM | 3312 | O   | THR | A | 420 | 10.141 | 23.312 | 65.300 | 1.00 | 18.82  |
| ATOM | 3313 | CB  | THR | A | 420 | 6.937  | 23.675 | 65.943 | 1.00 | 20.81  |
| ATOM | 3314 | OG1 | THR | A | 420 | 7.279  | 22.307 | 65.888 | 1.00 | 17.35  |
| ATOM | 3315 | CG2 | THR | A | 420 | 5.652  | 23.905 | 65.170 | 1.00 | 17.66  |
| ATOM | 3316 | N   | THR | A | 421 | 9.509  | 24.230 | 67.279 | 1.00 | 15.44  |
| ATOM | 3317 | CA  | THR | A | 421 | 10.627 | 23.719 | 68.062 | 1.00 | 14.71  |
| ATOM | 3318 | C   | THR | A | 421 | 10.714 | 22.185 | 67.921 | 1.00 | 19.15  |
| ATOM | 3319 | O   | THR | A | 421 | 11.801 | 21.642 | 67.832 | 1.00 | 18.94  |
| ATOM | 3320 | CB  | THR | A | 421 | 10.389 | 24.091 | 69.534 | 1.00 | 18.57  |
| ATOM | 3321 | OG1 | THR | A | 421 | 10.496 | 25.501 | 69.612 | 1.00 | 16.52  |
| ATOM | 3322 | CG2 | THR | A | 421 | 11.377 | 23.368 | 70.456 | 1.00 | 15.83  |
| ATOM | 3323 | N   | ASP | A | 422 | 9.580  | 21.463 | 67.890 | 1.00 | 15.92  |
| ATOM | 3324 | CA  | ASP | A | 422 | 9.659  | 19.986 | 67.722 | 1.00 | 14.54  |
| ATOM | 3325 | C   | ASP | A | 422 | 10.272 | 19.580 | 66.359 | 1.00 | 21.58  |
| ATOM | 3326 | O   | ASP | A | 422 | 11.048 | 18.588 | 66.225 | 1.00 | 20.31  |
| ATOM | 3327 | CB  | ASP | A | 422 | 8.314  | 19.238 | 67.909 | 1.00 | 14.53  |
| ATOM | 3328 | CG  | ASP | A | 422 | 8.560  | 17.737 | 67.831 | 1.00 | 19.43  |
| ATOM | 3329 | OD1 | ASP | A | 422 | 9.323  | 17.129 | 68.596 | 1.00 | 16.06  |
| ATOM | 3330 | OD2 | ASP | A | 422 | 7.911  | 17.117 | 66.852 | 1.00 | 21.53  |
| ATOM | 3331 | N   | ASP | A | 423 | 9.918  | 20.353 | 65.322 | 1.00 | 19.09  |
| ATOM | 3332 | CA  | ASP | A | 423 | 10.495 | 20.082 | 63.995 | 1.00 | 17.88  |
| ATOM | 3333 | C   | ASP | A | 423 | 12.013 | 20.170 | 64.096 | 1.00 | 19.57  |
| ATOM | 3334 | O   | ASP | A | 423 | 12.765 | 19.301 | 63.637 | 1.00 | 19.33  |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 3335 | CB  | ASP | A | 423 | 9.958  | 21.045 | 62.912 | 1.00 | 17.74 |
| ATOM | 3336 | CG  | ASP | A | 423 | 8.504  | 20.825 | 62.618 | 1.00 | 23.90 |
| ATOM | 3337 | OD1 | ASP | A | 423 | 8.010  | 19.730 | 62.614 | 1.00 | 31.78 |
| ATOM | 3338 | OD2 | ASP | A | 423 | 7.820  | 21.911 | 62.423 | 1.00 | 23.23 |
| ATOM | 3339 | N   | TRP | A | 424 | 12.459 | 21.248 | 64.730 | 1.00 | 15.04 |
| ATOM | 3340 | CA  | TRP | A | 424 | 13.889 | 21.495 | 64.920 | 1.00 | 15.04 |
| ATOM | 3341 | C   | TRP | A | 424 | 14.584 | 20.406 | 65.724 | 1.00 | 20.40 |
| ATOM | 3342 | O   | TRP | A | 424 | 15.596 | 19.843 | 65.336 | 1.00 | 17.34 |
| ATOM | 3343 | CB  | TRP | A | 424 | 14.071 | 22.831 | 65.642 | 1.00 | 15.30 |
| ATOM | 3344 | CG  | TRP | A | 424 | 15.484 | 23.055 | 66.071 | 1.00 | 16.43 |
| ATOM | 3345 | CD1 | TRP | A | 424 | 16.492 | 23.579 | 65.329 | 1.00 | 18.57 |
| ATOM | 3346 | CD2 | TRP | A | 424 | 16.018 | 22.769 | 67.349 | 1.00 | 15.38 |
| ATOM | 3347 | NE1 | TRP | A | 424 | 17.628 | 23.617 | 66.064 | 1.00 | 16.29 |
| ATOM | 3348 | CE2 | TRP | A | 424 | 17.370 | 23.117 | 67.308 | 1.00 | 16.11 |
| ATOM | 3349 | CE3 | TRP | A | 424 | 15.469 | 22.258 | 68.508 | 1.00 | 16.08 |
| ATOM | 3350 | CZ2 | TRP | A | 424 | 18.190 | 22.968 | 68.407 | 1.00 | 15.49 |
| ATOM | 3351 | CZ3 | TRP | A | 424 | 16.279 | 22.113 | 69.613 | 1.00 | 17.94 |
| ATOM | 3352 | CH2 | TRP | A | 424 | 17.627 | 22.474 | 69.563 | 1.00 | 18.84 |
| ATOM | 3353 | N   | LYS | A | 425 | 14.020 | 20.075 | 66.877 | 1.00 | 16.42 |
| ATOM | 3354 | CA  | LYS | A | 425 | 14.614 | 19.058 | 67.725 | 1.00 | 16.03 |
| ATOM | 3355 | C   | LYS | A | 425 | 14.518 | 17.671 | 67.082 | 1.00 | 19.39 |
| ATOM | 3356 | O   | LYS | A | 425 | 15.424 | 16.840 | 67.224 | 1.00 | 15.23 |
| ATOM | 3357 | CB  | LYS | A | 425 | 13.933 | 19.094 | 69.083 | 1.00 | 19.23 |
| ATOM | 3358 | CG  | LYS | A | 425 | 14.671 | 18.368 | 70.197 | 1.00 | 20.25 |
| ATOM | 3359 | CD  | LYS | A | 425 | 13.968 | 18.523 | 71.536 | 1.00 | 18.98 |
| ATOM | 3360 | CE  | LYS | A | 425 | 13.745 | 17.195 | 72.227 | 1.00 | 26.47 |
| ATOM | 3361 | NZ  | LYS | A | 425 | 12.642 | 16.425 | 71.626 | 1.00 | 29.32 |
| ATOM | 3362 | N   | ASP | A | 426 | 13.393 | 17.399 | 66.391 | 1.00 | 14.97 |
| ATOM | 3363 | CA  | ASP | A | 426 | 13.265 | 16.085 | 65.778 | 1.00 | 16.78 |
| ATOM | 3364 | C   | ASP | A | 426 | 14.386 | 15.932 | 64.720 | 1.00 | 24.04 |
| ATOM | 3365 | O   | ASP | A | 426 | 15.006 | 14.882 | 64.587 | 1.00 | 24.93 |
| ATOM | 3366 | CB  | ASP | A | 426 | 11.825 | 15.858 | 65.192 | 1.00 | 16.86 |
| ATOM | 3367 | CG  | ASP | A | 426 | 10.763 | 15.617 | 66.260 | 1.00 | 20.58 |
| ATOM | 3368 | OD1 | ASP | A | 426 | 10.993 | 15.457 | 67.440 | 1.00 | 19.54 |
| ATOM | 3369 | OD2 | ASP | A | 426 | 9.527  | 15.680 | 65.838 | 1.00 | 16.03 |
| ATOM | 3370 | N   | PHE | A | 427 | 14.649 | 17.012 | 63.971 | 1.00 | 17.98 |
| ATOM | 3371 | CA  | PHE | A | 427 | 15.683 | 16.995 | 62.927 | 1.00 | 18.47 |
| ATOM | 3372 | C   | PHE | A | 427 | 17.098 | 16.855 | 63.516 | 1.00 | 21.82 |
| ATOM | 3373 | O   | PHE | A | 427 | 17.966 | 16.117 | 63.064 | 1.00 | 20.65 |
| ATOM | 3374 | CB  | PHE | A | 427 | 15.567 | 18.226 | 62.012 | 1.00 | 17.69 |
| ATOM | 3375 | CG  | PHE | A | 427 | 16.598 | 18.171 | 60.945 | 1.00 | 18.08 |
| ATOM | 3376 | CD1 | PHE | A | 427 | 16.536 | 17.192 | 59.953 | 1.00 | 22.20 |
| ATOM | 3377 | CD2 | PHE | A | 427 | 17.673 | 19.058 | 60.951 | 1.00 | 20.78 |
| ATOM | 3378 | CE1 | PHE | A | 427 | 17.514 | 17.125 | 58.957 | 1.00 | 22.24 |
| ATOM | 3379 | CE2 | PHE | A | 427 | 18.659 | 19.007 | 59.965 | 1.00 | 23.56 |
| ATOM | 3380 | CZ  | PHE | A | 427 | 18.575 | 18.032 | 58.967 | 1.00 | 20.58 |
| ATOM | 3381 | N   | LEU | A | 428 | 17.323 | 17.575 | 64.567 | 1.00 | 16.49 |
| ATOM | 3382 | CA  | LEU | A | 428 | 18.582 | 17.512 | 65.258 | 1.00 | 17.57 |
| ATOM | 3383 | C   | LEU | A | 428 | 18.888 | 16.044 | 65.591 | 1.00 | 21.61 |
| ATOM | 3384 | O   | LEU | A | 428 | 19.995 | 15.562 | 65.387 | 1.00 | 22.21 |
| ATOM | 3385 | CB  | LEU | A | 428 | 18.467 | 18.372 | 66.573 | 1.00 | 18.03 |
| ATOM | 3386 | CG  | LEU | A | 428 | 19.727 | 18.463 | 67.424 | 1.00 | 22.98 |
| ATOM | 3387 | CD1 | LEU | A | 428 | 20.718 | 19.469 | 66.840 | 1.00 | 23.48 |
| ATOM | 3388 | CD2 | LEU | A | 428 | 19.347 | 18.859 | 68.843 | 1.00 | 19.42 |
| ATOM | 3389 | N   | TYR | A | 429 | 17.888 | 15.317 | 66.124 | 1.00 | 17.99 |
| ATOM | 3390 | CA  | TYR | A | 429 | 18.108 | 13.928 | 66.468 | 1.00 | 17.92 |
| ATOM | 3391 | C   | TYR | A | 429 | 18.317 | 13.083 | 65.234 | 1.00 | 20.04 |
| ATOM | 3392 | O   | TYR | A | 429 | 19.028 | 12.089 | 65.222 | 1.00 | 21.75 |



|      |      |     |     |   |     |        |        |        |      |        |
|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
| ATOM | 3393 | CB  | TYR | A | 429 | 16.930 | 13.365 | 67.228 | 1.00 | 16.70  |
| ATOM | 3394 | CG  | TYR | A | 429 | 17.129 | 13.527 | 68.694 | 1.00 | 19.75  |
| ATOM | 3395 | CD1 | TYR | A | 429 | 16.871 | 14.745 | 69.339 | 1.00 | 22.56  |
| ATOM | 3396 | CD2 | TYR | A | 429 | 17.551 | 12.436 | 69.450 | 1.00 | 19.39  |
| ATOM | 3397 | CE1 | TYR | A | 429 | 17.013 | 14.880 | 70.723 | 1.00 | 20.62  |
| ATOM | 3398 | CE2 | TYR | A | 429 | 17.719 | 12.555 | 70.827 | 1.00 | 19.33  |
| ATOM | 3399 | CZ  | TYR | A | 429 | 17.447 | 13.772 | 71.460 | 1.00 | 28.34  |
| ATOM | 3400 | OH  | TYR | A | 429 | 17.605 | 13.861 | 72.827 | 1.00 | 21.99  |
| ATOM | 3401 | N   | SER | A | 430 | 17.680 | 13.480 | 64.186 | 1.00 | 21.12  |
| ATOM | 3402 | CA  | SER | A | 430 | 17.814 | 12.754 | 62.966 | 1.00 | 22.17  |
| ATOM | 3403 | C   | SER | A | 430 | 19.202 | 12.960 | 62.417 | 1.00 | 27.73  |
| ATOM | 3404 | O   | SER | A | 430 | 19.905 | 12.020 | 62.037 | 1.00 | 29.03  |
| ATOM | 3405 | CB  | SER | A | 430 | 16.798 | 13.249 | 61.972 | 1.00 | 25.53  |
| ATOM | 3406 | OG  | SER | A | 430 | 16.768 | 12.307 | 60.941 | 1.00 | 38.11  |
| ATOM | 3407 | N   | TYR | A | 431 | 19.606 | 14.213 | 62.366 | 1.00 | 20.64  |
| ATOM | 3408 | CA  | TYR | A | 431 | 20.940 | 14.525 | 61.861 | 1.00 | 18.79  |
| ATOM | 3409 | C   | TYR | A | 431 | 22.067 | 13.832 | 62.650 | 1.00 | 28.08  |
| ATOM | 3410 | O   | TYR | A | 431 | 22.985 | 13.217 | 62.090 | 1.00 | 27.29  |
| ATOM | 3411 | CB  | TYR | A | 431 | 21.155 | 16.047 | 61.853 | 1.00 | 18.96  |
| ATOM | 3412 | CG  | TYR | A | 431 | 22.451 | 16.469 | 61.216 | 1.00 | 21.07  |
| ATOM | 3413 | CD1 | TYR | A | 431 | 22.515 | 16.652 | 59.834 | 1.00 | 22.11  |
| ATOM | 3414 | CD2 | TYR | A | 431 | 23.591 | 16.703 | 61.991 | 1.00 | 21.91  |
| ATOM | 3415 | CE1 | TYR | A | 431 | 23.710 | 17.020 | 59.217 | 1.00 | 21.48  |
| ATOM | 3416 | CE2 | TYR | A | 431 | 24.794 | 17.077 | 61.391 | 1.00 | 20.59  |
| ATOM | 3417 | CZ  | TYR | A | 431 | 24.845 | 17.237 | 60.002 | 1.00 | 26.37  |
| ATOM | 3418 | OH  | TYR | A | 431 | 26.023 | 17.606 | 59.384 | 1.00 | 25.96  |
| ATOM | 3419 | N   | PHE | A | 432 | 22.000 | 13.968 | 63.976 | 1.00 | 20.75  |
| ATOM | 3420 | CA  | PHE | A | 432 | 22.978 | 13.412 | 64.899 | 1.00 | 21.17  |
| ATOM | 3421 | C   | PHE | A | 432 | 22.574 | 12.027 | 65.391 | 1.00 | 29.42  |
| ATOM | 3422 | O   | PHE | A | 432 | 22.628 | 11.709 | 66.609 | 1.00 | 27.60  |
| ATOM | 3423 | CB  | PHE | A | 432 | 23.221 | 14.370 | 66.082 | 1.00 | 21.99  |
| ATOM | 3424 | CG  | PHE | A | 432 | 23.937 | 15.632 | 65.661 | 1.00 | 22.27  |
| ATOM | 3425 | CD1 | PHE | A | 432 | 25.310 | 15.611 | 65.413 | 1.00 | 23.51  |
| ATOM | 3426 | CD2 | PHE | A | 432 | 23.267 | 16.844 | 65.511 | 1.00 | 25.91  |
| ATOM | 3427 | CE1 | PHE | A | 432 | 26.017 | 16.751 | 65.038 | 1.00 | 23.71  |
| ATOM | 3428 | CE2 | PHE | A | 432 | 23.964 | 17.997 | 65.137 | 1.00 | 28.53  |
| ATOM | 3429 | CZ  | PHE | A | 432 | 25.337 | 17.958 | 64.903 | 1.00 | 24.21  |
| ATOM | 3430 | N   | LYS | A | 433 | 22.176 | 11.202 | 64.418 | 1.00 | 29.48  |
| ATOM | 3431 | CA  | LYS | A | 433 | 21.750 | 9.871  | 64.741 | 1.00 | 31.50  |
| ATOM | 3432 | C   | LYS | A | 433 | 22.772 | 9.105  | 65.542 | 1.00 | 38.53  |
| ATOM | 3433 | O   | LYS | A | 433 | 22.434 | 8.352  | 66.461 | 1.00 | 40.17  |
| ATOM | 3434 | CB  | LYS | A | 433 | 21.217 | 9.082  | 63.568 | 1.00 | 33.47  |
| ATOM | 3435 | CG  | LYS | A | 433 | 22.089 | 9.099  | 62.332 | 1.00 | 49.54  |
| ATOM | 3436 | CD  | LYS | A | 433 | 21.366 | 8.440  | 61.155 | 1.00 | 84.50  |
| ATOM | 3437 | CE  | LYS | A | 433 | 22.280 | 7.745  | 60.138 | 1.00 | 100.00 |
| ATOM | 3438 | NZ  | LYS | A | 433 | 23.098 | 6.630  | 60.676 | 1.00 | 100.00 |
| ATOM | 3439 | N   | ASP | A | 434 | 24.026 | 9.336  | 65.208 | 1.00 | 35.45  |
| ATOM | 3440 | CA  | ASP | A | 434 | 25.124 | 8.653  | 65.881 | 1.00 | 37.23  |
| ATOM | 3441 | C   | ASP | A | 434 | 25.525 | 9.192  | 67.245 | 1.00 | 38.69  |
| ATOM | 3442 | O   | ASP | A | 434 | 26.416 | 8.654  | 67.902 | 1.00 | 39.17  |
| ATOM | 3443 | CB  | ASP | A | 434 | 26.314 | 8.470  | 64.928 | 1.00 | 41.50  |
| ATOM | 3444 | CG  | ASP | A | 434 | 25.890 | 7.728  | 63.692 | 1.00 | 67.13  |
| ATOM | 3445 | OD1 | ASP | A | 434 | 25.175 | 6.717  | 63.728 | 1.00 | 67.36  |
| ATOM | 3446 | OD2 | ASP | A | 434 | 26.315 | 8.303  | 62.586 | 1.00 | 84.58  |
| ATOM | 3447 | N   | LYS | A | 435 | 24.853 | 10.245 | 67.689 | 1.00 | 32.08  |
| ATOM | 3448 | CA  | LYS | A | 435 | 25.162 | 10.821 | 68.969 | 1.00 | 29.32  |
| ATOM | 3449 | C   | LYS | A | 435 | 23.929 | 10.964 | 69.810 | 1.00 | 29.59  |
| ATOM | 3450 | O   | LYS | A | 435 | 23.900 | 11.671 | 70.787 | 1.00 | 32.10  |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 3451 | CB  | LYS | A | 435 | 25.898 | 12.127 | 68.804 | 1.00 | 33.40 |
| ATOM | 3452 | CG  | LYS | A | 435 | 27.071 | 12.016 | 67.829 | 1.00 | 32.88 |
| ATOM | 3453 | CD  | LYS | A | 435 | 27.667 | 13.366 | 67.474 | 1.00 | 38.14 |
| ATOM | 3454 | CE  | LYS | A | 435 | 29.124 | 13.505 | 67.880 | 1.00 | 48.06 |
| ATOM | 3455 | NZ  | LYS | A | 435 | 29.892 | 14.457 | 67.044 | 1.00 | 38.96 |
| ATOM | 3456 | N   | VAL | A | 436 | 22.890 | 10.278 | 69.418 | 1.00 | 26.88 |
| ATOM | 3457 | CA  | VAL | A | 436 | 21.645 | 10.309 | 70.163 | 1.00 | 29.00 |
| ATOM | 3458 | C   | VAL | A | 436 | 21.929 | 10.232 | 71.659 | 1.00 | 34.17 |
| ATOM | 3459 | O   | VAL | A | 436 | 21.263 | 10.835 | 72.511 | 1.00 | 32.94 |
| ATOM | 3460 | CB  | VAL | A | 436 | 20.773 | 9.138  | 69.695 | 1.00 | 35.31 |
| ATOM | 3461 | CG1 | VAL | A | 436 | 19.623 | 8.885  | 70.644 | 1.00 | 34.86 |
| ATOM | 3462 | CG2 | VAL | A | 436 | 20.210 | 9.448  | 68.314 | 1.00 | 35.95 |
| ATOM | 3463 | N   | ASP | A | 437 | 22.955 | 9.464  | 71.974 | 1.00 | 33.59 |
| ATOM | 3464 | CA  | ASP | A | 437 | 23.360 | 9.292  | 73.340 | 1.00 | 37.03 |
| ATOM | 3465 | C   | ASP | A | 437 | 23.794 | 10.594 | 73.986 | 1.00 | 39.40 |
| ATOM | 3466 | O   | ASP | A | 437 | 23.501 | 10.851 | 75.162 | 1.00 | 39.71 |
| ATOM | 3467 | CB  | ASP | A | 437 | 24.406 | 8.189  | 73.488 | 1.00 | 40.58 |
| ATOM | 3468 | CG  | ASP | A | 437 | 23.712 | 6.868  | 73.551 | 1.00 | 70.66 |
| ATOM | 3469 | OD1 | ASP | A | 437 | 22.493 | 6.763  | 73.671 | 1.00 | 70.63 |
| ATOM | 3470 | OD2 | ASP | A | 437 | 24.546 | 5.856  | 73.445 | 1.00 | 91.48 |
| ATOM | 3471 | N   | VAL | A | 438 | 24.495 | 11.400 | 73.200 | 1.00 | 33.72 |
| ATOM | 3472 | CA  | VAL | A | 438 | 24.945 | 12.698 | 73.657 | 1.00 | 34.65 |
| ATOM | 3473 | C   | VAL | A | 438 | 23.735 | 13.621 | 73.735 | 1.00 | 33.57 |
| ATOM | 3474 | O   | VAL | A | 438 | 23.536 | 14.325 | 74.704 | 1.00 | 34.91 |
| ATOM | 3475 | CB  | VAL | A | 438 | 26.034 | 13.287 | 72.758 | 1.00 | 37.55 |
| ATOM | 3476 | CG1 | VAL | A | 438 | 26.503 | 14.626 | 73.299 | 1.00 | 34.71 |
| ATOM | 3477 | CG2 | VAL | A | 438 | 27.208 | 12.318 | 72.709 | 1.00 | 38.05 |
| ATOM | 3478 | N   | LEU | A | 439 | 22.903 | 13.588 | 72.712 | 1.00 | 24.40 |
| ATOM | 3479 | CA  | LEU | A | 439 | 21.721 | 14.414 | 72.719 | 1.00 | 22.32 |
| ATOM | 3480 | C   | LEU | A | 439 | 20.834 | 14.099 | 73.924 | 1.00 | 26.48 |
| ATOM | 3481 | O   | LEU | A | 439 | 20.191 | 14.942 | 74.529 | 1.00 | 22.38 |
| ATOM | 3482 | CB  | LEU | A | 439 | 20.933 | 14.276 | 71.421 | 1.00 | 20.57 |
| ATOM | 3483 | CG  | LEU | A | 439 | 21.576 | 14.997 | 70.230 | 1.00 | 23.44 |
| ATOM | 3484 | CD1 | LEU | A | 439 | 20.906 | 14.546 | 68.949 | 1.00 | 21.22 |
| ATOM | 3485 | CD2 | LEU | A | 439 | 21.448 | 16.504 | 70.377 | 1.00 | 26.40 |
| ATOM | 3486 | N   | ASN | A | 440 | 20.812 | 12.857 | 74.328 | 1.00 | 28.97 |
| ATOM | 3487 | CA  | ASN | A | 440 | 19.989 | 12.526 | 75.468 | 1.00 | 30.65 |
| ATOM | 3488 | C   | ASN | A | 440 | 20.485 | 13.059 | 76.815 | 1.00 | 36.08 |
| ATOM | 3489 | O   | ASN | A | 440 | 19.797 | 12.963 | 77.840 | 1.00 | 35.25 |
| ATOM | 3490 | CB  | ASN | A | 440 | 19.572 | 11.051 | 75.500 | 1.00 | 32.98 |
| ATOM | 3491 | CG  | ASN | A | 440 | 18.715 | 10.673 | 74.297 | 1.00 | 44.08 |
| ATOM | 3492 | OD1 | ASN | A | 440 | 18.880 | 9.598  | 73.713 | 1.00 | 45.17 |
| ATOM | 3493 | ND2 | ASN | A | 440 | 17.787 | 11.540 | 73.932 | 1.00 | 28.22 |
| ATOM | 3494 | N   | GLN | A | 441 | 21.671 | 13.638 | 76.817 | 1.00 | 31.53 |
| ATOM | 3495 | CA  | GLN | A | 441 | 22.229 | 14.187 | 78.039 | 1.00 | 31.77 |
| ATOM | 3496 | C   | GLN | A | 441 | 21.697 | 15.567 | 78.287 | 1.00 | 29.73 |
| ATOM | 3497 | O   | GLN | A | 441 | 21.898 | 16.161 | 79.338 | 1.00 | 29.53 |
| ATOM | 3498 | CB  | GLN | A | 441 | 23.761 | 14.354 | 77.925 | 1.00 | 34.83 |
| ATOM | 3499 | CG  | GLN | A | 441 | 24.547 | 13.034 | 77.744 | 1.00 | 58.52 |
| ATOM | 3500 | CD  | GLN | A | 441 | 25.923 | 13.263 | 77.141 | 1.00 | 89.10 |
| ATOM | 3501 | OE1 | GLN | A | 441 | 26.427 | 14.407 | 77.102 | 1.00 | 88.57 |
| ATOM | 3502 | NE2 | GLN | A | 441 | 26.520 | 12.176 | 76.643 | 1.00 | 77.72 |
| ATOM | 3503 | N   | VAL | A | 442 | 21.060 | 16.102 | 77.281 | 1.00 | 24.12 |
| ATOM | 3504 | CA  | VAL | A | 442 | 20.559 | 17.455 | 77.403 | 1.00 | 21.42 |
| ATOM | 3505 | C   | VAL | A | 442 | 19.291 | 17.500 | 78.203 | 1.00 | 24.42 |
| ATOM | 3506 | O   | VAL | A | 442 | 18.413 | 16.685 | 77.985 | 1.00 | 24.57 |
| ATOM | 3507 | CB  | VAL | A | 442 | 20.290 | 18.001 | 76.008 | 1.00 | 24.29 |
| ATOM | 3508 | CG1 | VAL | A | 442 | 19.812 | 19.440 | 76.055 | 1.00 | 20.29 |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 3509 | CG2 | VAL | A | 442 | 21.533 | 17.877 | 75.146 | 1.00 | 24.17 |
| ATOM | 3510 | N   | ASP | A | 443 | 19.182 | 18.455 | 79.117 | 1.00 | 20.38 |
| ATOM | 3511 | CA  | ASP | A | 443 | 17.949 | 18.592 | 79.885 | 1.00 | 18.65 |
| ATOM | 3512 | C   | ASP | A | 443 | 17.033 | 19.466 | 79.007 | 1.00 | 20.56 |
| ATOM | 3513 | O   | ASP | A | 443 | 16.908 | 20.685 | 79.188 | 1.00 | 19.27 |
| ATOM | 3514 | CB  | ASP | A | 443 | 18.268 | 19.278 | 81.234 | 1.00 | 17.23 |
| ATOM | 3515 | CG  | ASP | A | 443 | 17.107 | 19.409 | 82.156 | 1.00 | 22.28 |
| ATOM | 3516 | OD1 | ASP | A | 443 | 15.962 | 19.193 | 81.821 | 1.00 | 25.25 |
| ATOM | 3517 | OD2 | ASP | A | 443 | 17.469 | 19.832 | 83.350 | 1.00 | 29.16 |
| ATOM | 3518 | N   | TRP | A | 444 | 16.444 | 18.841 | 77.991 | 1.00 | 18.61 |
| ATOM | 3519 | CA  | TRP | A | 444 | 15.589 | 19.555 | 77.044 | 1.00 | 19.23 |
| ATOM | 3520 | C   | TRP | A | 444 | 14.447 | 20.283 | 77.739 | 1.00 | 22.43 |
| ATOM | 3521 | O   | TRP | A | 444 | 14.106 | 21.378 | 77.357 | 1.00 | 20.87 |
| ATOM | 3522 | CB  | TRP | A | 444 | 15.014 | 18.571 | 75.999 | 1.00 | 16.26 |
| ATOM | 3523 | CG  | TRP | A | 444 | 16.075 | 18.037 | 75.111 | 1.00 | 17.37 |
| ATOM | 3524 | CD1 | TRP | A | 444 | 16.577 | 16.760 | 75.075 | 1.00 | 20.43 |
| ATOM | 3525 | CD2 | TRP | A | 444 | 16.766 | 18.764 | 74.121 | 1.00 | 17.48 |
| ATOM | 3526 | NE1 | TRP | A | 444 | 17.571 | 16.654 | 74.130 | 1.00 | 16.65 |
| ATOM | 3527 | CE2 | TRP | A | 444 | 17.691 | 17.869 | 73.509 | 1.00 | 18.92 |
| ATOM | 3528 | CE3 | TRP | A | 444 | 16.684 | 20.086 | 73.666 | 1.00 | 19.00 |
| ATOM | 3529 | CZ2 | TRP | A | 444 | 18.513 | 18.295 | 72.461 | 1.00 | 19.33 |
| ATOM | 3530 | CZ3 | TRP | A | 444 | 17.515 | 20.495 | 72.617 | 1.00 | 19.57 |
| ATOM | 3531 | CH2 | TRP | A | 444 | 18.434 | 19.619 | 72.044 | 1.00 | 19.75 |
| ATOM | 3532 | N   | ASN | A | 445 | 13.826 | 19.632 | 78.740 | 1.00 | 20.30 |
| ATOM | 3533 | CA  | ASN | A | 445 | 12.706 | 20.224 | 79.463 | 1.00 | 20.89 |
| ATOM | 3534 | C   | ASN | A | 445 | 13.077 | 21.554 | 80.087 | 1.00 | 20.91 |
| ATOM | 3535 | O   | ASN | A | 445 | 12.322 | 22.527 | 80.040 | 1.00 | 21.65 |
| ATOM | 3536 | CB  | ASN | A | 445 | 12.137 | 19.320 | 80.595 | 1.00 | 21.46 |
| ATOM | 3537 | CG  | ASN | A | 445 | 11.115 | 20.025 | 81.495 | 1.00 | 39.63 |
| ATOM | 3538 | OD1 | ASN | A | 445 | 11.392 | 20.355 | 82.657 | 1.00 | 39.64 |
| ATOM | 3539 | ND2 | ASN | A | 445 | 9.925  | 20.274 | 80.974 | 1.00 | 29.20 |
| ATOM | 3540 | N   | ALA | A | 446 | 14.222 | 21.569 | 80.734 | 1.00 | 18.04 |
| ATOM | 3541 | CA  | ALA | A | 446 | 14.639 | 22.777 | 81.382 | 1.00 | 17.64 |
| ATOM | 3542 | C   | ALA | A | 446 | 14.981 | 23.810 | 80.348 | 1.00 | 21.98 |
| ATOM | 3543 | O   | ALA | A | 446 | 14.533 | 24.966 | 80.400 | 1.00 | 22.74 |
| ATOM | 3544 | CB  | ALA | A | 446 | 15.792 | 22.515 | 82.324 | 1.00 | 18.03 |
| ATOM | 3545 | N   | TRP | A | 447 | 15.760 | 23.390 | 79.386 | 1.00 | 14.45 |
| ATOM | 3546 | CA  | TRP | A | 447 | 16.152 | 24.344 | 78.368 | 1.00 | 15.22 |
| ATOM | 3547 | C   | TRP | A | 447 | 14.989 | 24.963 | 77.589 | 1.00 | 17.91 |
| ATOM | 3548 | O   | TRP | A | 447 | 15.015 | 26.157 | 77.286 | 1.00 | 16.55 |
| ATOM | 3549 | CB  | TRP | A | 447 | 17.136 | 23.694 | 77.357 | 1.00 | 16.85 |
| ATOM | 3550 | CG  | TRP | A | 447 | 18.610 | 23.756 | 77.719 | 1.00 | 20.22 |
| ATOM | 3551 | CD1 | TRP | A | 447 |        |        |        |      |       |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 3567 | N   | TYR | A | 449 | 11.365 | 24.630 | 78.287 | 1.00 | 14.33 |
| ATOM | 3568 | CA  | TYR | A | 449 | 10.196 | 25.053 | 79.029 | 1.00 | 14.18 |
| ATOM | 3569 | C   | TYR | A | 449 | 10.411 | 25.677 | 80.383 | 1.00 | 24.16 |
| ATOM | 3570 | O   | TYR | A | 449 | 9.453  | 26.169 | 80.973 | 1.00 | 31.60 |
| ATOM | 3571 | CB  | TYR | A | 449 | 9.242  | 23.846 | 79.133 | 1.00 | 14.78 |
| ATOM | 3572 | CG  | TYR | A | 449 | 9.181  | 23.150 | 77.809 | 1.00 | 18.85 |
| ATOM | 3573 | CD1 | TYR | A | 449 | 8.803  | 23.864 | 76.673 | 1.00 | 22.43 |
| ATOM | 3574 | CD2 | TYR | A | 449 | 9.544  | 21.811 | 77.678 | 1.00 | 21.55 |
| ATOM | 3575 | CE1 | TYR | A | 449 | 8.780  | 23.284 | 75.406 | 1.00 | 23.44 |
| ATOM | 3576 | CE2 | TYR | A | 449 | 9.524  | 21.204 | 76.421 | 1.00 | 24.76 |
| ATOM | 3577 | CZ  | TYR | A | 449 | 9.139  | 21.940 | 75.297 | 1.00 | 30.93 |
| ATOM | 3578 | OH  | TYR | A | 449 | 9.104  | 21.340 | 74.074 | 1.00 | 32.94 |
| ATOM | 3579 | N   | SER | A | 450 | 11.632 | 25.666 | 80.922 | 1.00 | 20.74 |
| ATOM | 3580 | CA  | SER | A | 450 | 11.805 | 26.273 | 82.232 | 1.00 | 19.22 |
| ATOM | 3581 | C   | SER | A | 450 | 12.173 | 27.745 | 82.136 | 1.00 | 19.24 |
| ATOM | 3582 | O   | SER | A | 450 | 12.873 | 28.169 | 81.232 | 1.00 | 16.93 |
| ATOM | 3583 | CB  | SER | A | 450 | 12.788 | 25.513 | 83.115 | 1.00 | 18.75 |
| ATOM | 3584 | OG  | SER | A | 450 | 12.355 | 24.182 | 83.271 | 1.00 | 19.76 |
| ATOM | 3585 | N   | PRO | A | 451 | 11.708 | 28.532 | 83.090 | 1.00 | 18.00 |
| ATOM | 3586 | CA  | PRO | A | 451 | 12.037 | 29.932 | 83.102 | 1.00 | 14.60 |
| ATOM | 3587 | C   | PRO | A | 451 | 13.417 | 30.093 | 83.732 | 1.00 | 19.79 |
| ATOM | 3588 | O   | PRO | A | 451 | 13.984 | 29.124 | 84.228 | 1.00 | 19.56 |
| ATOM | 3589 | CB  | PRO | A | 451 | 11.037 | 30.565 | 84.057 | 1.00 | 15.55 |
| ATOM | 3590 | CG  | PRO | A | 451 | 10.705 | 29.459 | 85.055 | 1.00 | 21.58 |
| ATOM | 3591 | CD  | PRO | A | 451 | 11.020 | 28.141 | 84.342 | 1.00 | 21.20 |
| ATOM | 3592 | N   | GLY | A | 452 | 13.928 | 31.341 | 83.724 | 1.00 | 17.89 |
| ATOM | 3593 | CA  | GLY | A | 452 | 15.202 | 31.665 | 84.338 | 1.00 | 18.57 |
| ATOM | 3594 | C   | GLY | A | 452 | 16.407 | 31.317 | 83.478 | 1.00 | 21.97 |
| ATOM | 3595 | O   | GLY | A | 452 | 16.290 | 31.071 | 82.276 | 1.00 | 21.83 |
| ATOM | 3596 | N   | LEU | A | 453 | 17.589 | 31.317 | 84.107 | 1.00 | 19.93 |
| ATOM | 3597 | CA  | LEU | A | 453 | 18.837 | 30.982 | 83.415 | 1.00 | 18.02 |
| ATOM | 3598 | C   | LEU | A | 453 | 18.793 | 29.544 | 82.986 | 1.00 | 16.18 |
| ATOM | 3599 | O   | LEU | A | 453 | 18.144 | 28.738 | 83.626 | 1.00 | 17.78 |
| ATOM | 3600 | CB  | LEU | A | 453 | 20.094 | 31.244 | 84.292 | 1.00 | 17.95 |
| ATOM | 3601 | CG  | LEU | A | 453 | 20.310 | 32.752 | 84.572 | 1.00 | 23.56 |
| ATOM | 3602 | CD1 | LEU | A | 453 | 21.420 | 32.994 | 85.574 | 1.00 | 22.35 |
| ATOM | 3603 | CD2 | LEU | A | 453 | 20.625 | 33.534 | 83.300 | 1.00 | 30.45 |
| ATOM | 3604 | N   | PRO | A | 454 | 19.484 | 29.235 | 81.905 | 1.00 | 13.25 |
| ATOM | 3605 | CA  | PRO | A | 454 | 19.535 | 27.899 | 81.411 | 1.00 | 15.46 |
| ATOM | 3606 | C   | PRO | A | 454 | 20.119 | 27.024 | 82.485 | 1.00 | 23.30 |
| ATOM | 3607 | O   | PRO | A | 454 | 20.815 | 27.513 | 83.353 | 1.00 | 23.78 |
| ATOM | 3608 | CB  | PRO | A | 454 | 20.495 | 27.948 | 80.237 | 1.00 | 17.39 |
| ATOM | 3609 | CG  | PRO | A | 454 | 20.556 | 29.378 | 79.823 | 1.00 | 18.14 |
| ATOM | 3610 | CD  | PRO | A | 454 | 20.075 | 30.206 | 80.977 | 1.00 | 13.32 |
| ATOM | 3611 | N   | PRO | A | 455 | 19.829 | 25.723 | 82.410 | 1.00 | 21.53 |
| ATOM | 3612 | CA  | PRO | A | 455 | 20.272 | 24.743 | 83.370 | 1.00 | 19.23 |
| ATOM | 3613 | C   | PRO | A | 455 | 21.770 | 24.549 | 83.389 | 1.00 | 25.57 |
| ATOM | 3614 | O   | PRO | A | 455 | 22.296 | 23.986 | 84.337 | 1.00 | 27.35 |
| ATOM | 3615 | CB  | PRO | A | 455 | 19.652 | 23.427 | 82.900 | 1.00 | 22.39 |
| ATOM | 3616 | CG  | PRO | A | 455 | 19.374 | 23.599 | 81.408 | 1.00 | 26.96 |
| ATOM | 3617 | CD  | PRO | A | 455 | 19.350 | 25.092 | 81.148 | 1.00 | 22.06 |
| ATOM | 3618 | N   | ILE | A | 456 | 22.447 | 24.964 | 82.326 | 1.00 | 23.73 |
| ATOM | 3619 | CA  | ILE | A | 456 | 23.899 | 24.830 | 82.174 | 1.00 | 23.23 |
| ATOM | 3620 | C   | ILE | A | 456 | 24.529 | 25.986 | 81.356 | 1.00 | 27.18 |
| ATOM | 3621 | O   | ILE | A | 456 | 23.978 | 26.449 | 80.360 | 1.00 | 24.63 |
| ATOM | 3622 | CB  | ILE | A | 456 | 24.307 | 23.478 | 81.556 | 1.00 | 25.34 |
| ATOM | 3623 | CG1 | ILE | A | 456 | 25.823 | 23.393 | 81.561 | 1.00 | 27.12 |
| ATOM | 3624 | CG2 | ILE | A | 456 | 23.869 | 23.383 | 80.104 | 1.00 | 22.88 |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 3625 | CD1 | ILE | A | 456 | 26.315 | 22.032 | 81.111 | 1.00 | 37.60 |
| ATOM | 3626 | N   | LYS | A | 457 | 25.703 | 26.440 | 81.796 | 1.00 | 23.16 |
| ATOM | 3627 | CA  | LYS | A | 457 | 26.410 | 27.503 | 81.125 | 1.00 | 19.98 |
| ATOM | 3628 | C   | LYS | A | 457 | 27.497 | 26.952 | 80.216 | 1.00 | 19.32 |
| ATOM | 3629 | O   | LYS | A | 457 | 28.321 | 26.142 | 80.606 | 1.00 | 20.28 |
| ATOM | 3630 | CB  | LYS | A | 457 | 27.017 | 28.412 | 82.169 | 1.00 | 18.35 |
| ATOM | 3631 | CG  | LYS | A | 457 | 27.630 | 29.654 | 81.540 | 1.00 | 19.13 |
| ATOM | 3632 | CD  | LYS | A | 457 | 28.040 | 30.704 | 82.573 | 1.00 | 13.39 |
| ATOM | 3633 | CE  | LYS | A | 457 | 28.595 | 31.975 | 81.976 | 1.00 | 19.02 |
| ATOM | 3634 | NZ  | LYS | A | 457 | 29.079 | 32.871 | 83.038 | 1.00 | 25.4  |
| ATOM | 3635 | N   | PRO | A | 458 | 27.510 | 27.368 | 78.980 | 1.00 | 17.25 |
| ATOM | 3636 | CA  | PRO | A | 458 | 28.561 | 26.873 | 78.092 | 1.00 | 16.78 |
| ATOM | 3637 | C   | PRO | A | 458 | 29.948 | 27.342 | 78.587 | 1.00 | 21.03 |
| ATOM | 3638 | O   | PRO | A | 458 | 30.098 | 28.121 | 79.548 | 1.00 | 18.45 |
| ATOM | 3639 | CB  | PRO | A | 458 | 28.291 | 27.537 | 76.706 | 1.00 | 15.89 |
| ATOM | 3640 | CG  | PRO | A | 458 | 26.889 | 28.090 | 76.751 | 1.00 | 18.86 |
| ATOM | 3641 | CD  | PRO | A | 458 | 26.514 | 28.209 | 78.240 | 1.00 | 15.44 |
| ATOM | 3642 | N   | ASN | A | 459 | 30.975 | 26.874 | 77.892 | 1.00 | 19.04 |
| ATOM | 3643 | CA  | ASN | A | 459 | 32.363 | 27.253 | 78.179 | 1.00 | 17.72 |
| ATOM | 3644 | C   | ASN | A | 459 | 32.713 | 28.426 | 77.277 | 1.00 | 21.16 |
| ATOM | 3645 | O   | ASN | A | 459 | 32.358 | 28.395 | 76.110 | 1.00 | 21.77 |
| ATOM | 3646 | CB  | ASN | A | 459 | 33.283 | 26.119 | 77.766 | 1.00 | 16.35 |
| ATOM | 3647 | CG  | ASN | A | 459 | 32.986 | 24.915 | 78.600 | 1.00 | 33.77 |
| ATOM | 3648 | OD1 | ASN | A | 459 | 32.711 | 25.054 | 79.801 | 1.00 | 32.94 |
| ATOM | 3649 | ND2 | ASN | A | 459 | 32.997 | 23.744 | 77.971 | 1.00 | 35.74 |
| ATOM | 3650 | N   | TYR | A | 460 | 33.391 | 29.456 | 77.813 | 1.00 | 18.66 |
| ATOM | 3651 | CA  | TYR | A | 460 | 33.753 | 30.635 | 77.038 | 1.00 | 18.11 |
| ATOM | 3652 | C   | TYR | A | 460 | 35.213 | 31.026 | 77.185 | 1.00 | 20.75 |
| ATOM | 3653 | O   | TYR | A | 460 | 35.741 | 31.119 | 78.307 | 1.00 | 18.62 |
| ATOM | 3654 | CB  | TYR | A | 460 | 32.976 | 31.904 | 77.478 | 1.00 | 18.18 |
| ATOM | 3655 | CG  | TYR | A | 460 | 31.478 | 31.810 | 77.386 | 1.00 | 17.73 |
| ATOM | 3656 | CD1 | TYR | A | 460 | 30.749 | 31.188 | 78.396 | 1.00 | 20.44 |
| ATOM | 3657 | CD2 | TYR | A | 460 | 30.794 | 32.337 | 76.292 | 1.00 | 16.25 |
| ATOM | 3658 | CE1 | TYR | A | 460 | 29.360 | 31.101 | 78.337 | 1.00 | 23.40 |
| ATOM | 3659 | CE2 | TYR | A | 460 | 29.404 | 32.232 | 76.198 | 1.00 | 14.35 |
| ATOM | 3660 | CZ  | TYR | A | 460 | 28.690 | 31.628 | 77.231 | 1.00 | 21.89 |
| ATOM | 3661 | OH  | TYR | A | 460 | 27.326 | 31.523 | 77.162 | 1.00 | 16.31 |
| ATOM | 3662 | N   | ASP | A | 461 | 35.842 | 31.343 | 76.046 | 1.00 | 19.66 |
| ATOM | 3663 | CA  | ASP | A | 461 | 37.212 | 31.809 | 76.095 | 1.00 | 18.27 |
| ATOM | 3664 | C   | ASP | A | 461 | 37.169 | 33.141 | 76.798 | 1.00 | 18.19 |
| ATOM | 3665 | O   | ASP | A | 461 | 36.188 | 33.860 | 76.643 | 1.00 | 18.93 |
| ATOM | 3666 | CB  | ASP | A | 461 | 37.798 | 31.934 | 74.697 | 1.00 | 23.01 |
| ATOM | 3667 | CG  | ASP | A | 461 | 39.212 |        |        |      |       |



|      |      |     |     |   |     |        |          |        |      |       |
|------|------|-----|-----|---|-----|--------|----------|--------|------|-------|
| ATOM | 3683 | OG1 | THR | A | 463 | 41.785 | 34.618   | 74.927 | 1.00 | 20.48 |
| ATOM | 3684 | CG2 | THR | A | 463 | 42.653 | 36.821   | 74.545 | 1.00 | 19.13 |
| ATOM | 3685 | N   | LEU | A | 464 | 39.500 | 38.305   | 75.582 | 1.00 | 17.78 |
| ATOM | 3686 | CA  | LEU | A | 464 | 39.123 | 39.732   | 75.548 | 1.00 | 19.02 |
| ATOM | 3687 | C   | LEU | A | 464 | 38.314 | 40.259   | 76.751 | 1.00 | 18.77 |
| ATOM | 3688 | O   | LEU | A | 464 | 38.250 | 41.450   | 77.001 | 1.00 | 21.30 |
| ATOM | 3689 | CB  | LEU | A | 464 | 38.360 | 40.033   | 74.245 | 1.00 | 20.69 |
| ATOM | 3690 | CG  | LEU | A | 464 | 39.213 | 39.688   | 73.006 | 1.00 | 27.61 |
| ATOM | 3691 | CD1 | LEU | A | 464 | 38.360 | 39.792   | 71.728 | 1.00 | 29.60 |
| ATOM | 3692 | CD2 | LEU | A | 464 | 40.427 | 40.619   | 72.898 | 1.00 | 21.71 |
| ATOM | 3693 | N   | THR | A | 465 | 37.674 | 39.353   | 77.479 | 1.00 | 15.92 |
| ATOM | 3694 | CA  | THR | A | 465 | 36.843 | 39.694   | 78.609 | 1.00 | 14.62 |
| ATOM | 3695 | C   | THR | A | 465 | 37.619 | 40.024   | 79.854 | 1.00 | 17.84 |
| ATOM | 3696 | O   | THR | A | 465 | 37.211 | 40.865   | 80.646 | 1.00 | 16.88 |
| ATOM | 3697 | CB  | THR | A | 465 | 35.871 | 38.550   | 78.901 | 1.00 | 21.80 |
| ATOM | 3698 | OG1 | THR | A | 465 | 35.073 | 38.342   | 77.759 | 1.00 | 18.69 |
| ATOM | 3699 | CG2 | THR | A | 465 | 34.956 | 38.944   | 80.041 | 1.00 | 25.42 |
| ATOM | 3700 | N   | ASN | A | 466 | 38.721 | 39.324   | 80.043 | 1.00 | 16.40 |
| ATOM | 3701 | CA  | ASN | A | 466 | 39.540 | 39.527   | 81.213 | 1.00 | 16.14 |
| ATOM | 3702 | C   | ASN | A | 466 | 39.836 | 40.996   | 81.525 | 1.00 | 19.38 |
| ATOM | 3703 | O   | ASN | A | 466 | 39.734 | 41.439   | 82.663 | 1.00 | 19.58 |
| ATOM | 3704 | CB  | ASN | A | 466 | 40.849 | 38.731   | 81.111 | 1.00 | 14.60 |
| ATOM | 3705 | CG  | ASN | A | 466 | 40.657 | 37.270   | 81.423 | 1.00 | 26.76 |
| ATOM | 3706 | OD1 | ASN | A | 466 | 41.408 | 36.403   | 80.963 | 1.00 | 25.03 |
| ATOM | 3707 | ND2 | ASN | A | 466 | 39.660 | 36.987   | 82.248 | 1.00 | 19.27 |
| ATOM | 3708 | N   | ALA | A | 467 | 40.235 | 41.789   | 80.553 | 1.00 | 15.87 |
| ATOM | 3709 | CA  | ALA | A | 467 | 40.531 | 43.172   | 80.894 | 1.00 | 13.57 |
| ATOM | 3710 | C   | ALA | A | 467 | 39.287 | 43.952   | 81.326 | 1.00 | 20.84 |
| ATOM | 3711 | O   | ALA | A | 467 | 39.354 | 44.894   | 82.135 | 1.00 | 20.42 |
| ATOM | 3712 | CB  | ALA | A | 467 | 41.227 | 43.871   | 79.761 | 1.00 | 13.94 |
| ATOM | 3713 | N   | CYS | A | 468 | 38.120 | 43.554   | 80.791 | 1.00 | 19.04 |
| ATOM | 3714 | CA  | CYS | A | 468 | 36.901 | 44.243   | 81.149 | 1.00 | 17.27 |
| ATOM | 3715 | C   | CYS | A | 468 | 36.537 | 43.974   | 82.585 | 1.00 | 17.05 |
| ATOM | 3716 | O   | CYS | A | 468 | 36.056 | 44.844   | 83.325 | 1.00 | 17.72 |
| ATOM | 3717 | CB  | CYS | A | 468 | 35.774 | 43.798   | 80.232 | 1.00 | 17.11 |
| ATOM | 3718 | SG  | CYS | A | 468 | 36.190 | 44.017   | 78.497 | 1.00 | 20.64 |
| ATOM | 3719 | N   | ILE | A | 469 | 36.760 | 42.727   | 82.956 | 1.00 | 14.28 |
| ATOM | 3720 | CA  | ILE | A | 469 | 36.466 | 42.270   | 84.287 | 1.00 | 13.17 |
| ATOM | 3721 | C   | ILE | A | 469 | 37.332 | 42.942   | 85.315 | 1.00 | 17.17 |
| ATOM | 3722 | O   | ILE | A | 469 | 36.873 | 43.371   | 86.379 | 1.00 | 16.23 |
| ATOM | 3723 | CB  | ILE | A | 469 | 36.609 | 40.788   | 84.347 | 1.00 | 16.75 |
| ATOM | 3724 | CG1 | ILE | A | 469 | 35.407 | 40.190   | 83.624 | 1.00 | 19.41 |
| ATOM | 3725 | CG2 | ILE | A | 469 | 36.602 | 40.402</ |        |      |       |



00122110 022659

|      |      |     |     |       |        |        |        |      |       |
|------|------|-----|-----|-------|--------|--------|--------|------|-------|
| ATOM | 3741 | CA  | SER | A 472 | 34.893 | 46.789 | 86.172 | 1.00 | 16.97 |
| ATOM | 3742 | C   | SER | A 472 | 34.991 | 46.475 | 87.679 | 1.00 | 18.47 |
| ATOM | 3743 | O   | SER | A 472 | 34.406 | 47.153 | 88.555 | 1.00 | 19.09 |
| ATOM | 3744 | CB  | SER | A 472 | 33.774 | 45.995 | 85.503 | 1.00 | 17.40 |
| ATOM | 3745 | OG  | SER | A 472 | 34.008 | 44.617 | 85.597 | 1.00 | 23.16 |
| ATOM | 3746 | N   | GLN | A 473 | 35.717 | 45.423 | 87.996 | 1.00 | 12.19 |
| ATOM | 3747 | CA  | GLN | A 473 | 35.819 | 45.089 | 89.379 | 1.00 | 12.48 |
| ATOM | 3748 | C   | GLN | A 473 | 36.518 | 46.171 | 90.135 | 1.00 | 15.41 |
| ATOM | 3749 | O   | GLN | A 473 | 36.151 | 46.482 | 91.277 | 1.00 | 15.83 |
| ATOM | 3750 | CB  | GLN | A 473 | 36.536 | 43.762 | 89.601 | 1.00 | 15.35 |
| ATOM | 3751 | CG  | GLN | A 473 | 35.633 | 42.544 | 89.397 | 1.00 | 28.01 |
| ATOM | 3752 | CD  | GLN | A 473 | 34.591 | 42.414 | 90.486 | 1.00 | 23.21 |
| ATOM | 3753 | OE1 | GLN | A 473 | 34.943 | 42.280 | 91.646 | 1.00 | 30.81 |
| ATOM | 3754 | NE2 | GLN | A 473 | 33.317 | 42.443 | 90.118 | 1.00 | 20.42 |
| ATOM | 3755 | N   | ARG | A 474 | 37.526 | 46.773 | 89.500 | 1.00 | 15.24 |
| ATOM | 3756 | CA  | ARG | A 474 | 38.237 | 47.862 | 90.194 | 1.00 | 16.28 |
| ATOM | 3757 | C   | ARG | A 474 | 37.329 | 49.021 | 90.504 | 1.00 | 20.39 |
| ATOM | 3758 | O   | ARG | A 474 | 37.435 | 49.652 | 91.553 | 1.00 | 17.27 |
| ATOM | 3759 | CB  | ARG | A 474 | 39.423 | 48.395 | 89.439 | 1.00 | 18.74 |
| ATOM | 3760 | CG  | ARG | A 474 | 40.550 | 47.374 | 89.293 | 1.00 | 26.58 |
| ATOM | 3761 | CD  | ARG | A 474 | 41.618 | 47.883 | 88.341 | 1.00 | 20.51 |
| ATOM | 3762 | NE  | ARG | A 474 | 41.969 | 49.292 | 88.607 | 1.00 | 23.54 |
| ATOM | 3763 | CZ  | ARG | A 474 | 42.633 | 50.045 | 87.715 | 1.00 | 36.01 |
| ATOM | 3764 | NH1 | ARG | A 474 | 42.999 | 49.538 | 86.533 | 1.00 | 25.73 |
| ATOM | 3765 | NH2 | ARG | A 474 | 42.952 | 51.314 | 88.008 | 1.00 | 20.34 |
| ATOM | 3766 | N   | TRP | A 475 | 36.431 | 49.339 | 89.585 | 1.00 | 13.75 |
| ATOM | 3767 | CA  | TRP | A 475 | 35.546 | 50.423 | 89.885 | 1.00 | 14.04 |
| ATOM | 3768 | C   | TRP | A 475 | 34.480 | 50.022 | 90.904 | 1.00 | 21.95 |
| ATOM | 3769 | O   | TRP | A 475 | 34.182 | 50.738 | 91.845 | 1.00 | 20.08 |
| ATOM | 3770 | CB  | TRP | A 475 | 34.902 | 50.918 | 88.643 | 1.00 | 14.34 |
| ATOM | 3771 | CG  | TRP | A 475 | 35.781 | 51.876 | 87.925 | 1.00 | 16.86 |
| ATOM | 3772 | CD1 | TRP | A 475 | 36.579 | 51.601 | 86.855 | 1.00 | 19.96 |
| ATOM | 3773 | CD2 | TRP | A 475 | 35.932 | 53.280 | 88.198 | 1.00 | 16.47 |
| ATOM | 3774 | NE1 | TRP | A 475 | 37.226 | 52.747 | 86.432 | 1.00 | 19.52 |
| ATOM | 3775 | CE2 | TRP | A 475 | 36.856 | 53.797 | 87.250 | 1.00 | 20.19 |
| ATOM | 3776 | CE3 | TRP | A 475 | 35.396 | 54.132 | 89.154 | 1.00 | 17.53 |
| ATOM | 3777 | CZ2 | TRP | A 475 | 37.225 | 55.156 | 87.232 | 1.00 | 18.93 |
| ATOM | 3778 | CZ3 | TRP | A 475 | 35.782 | 55.462 | 89.148 | 1.00 | 19.08 |
| ATOM | 3779 | CH2 | TRP | A 475 | 36.681 | 55.963 | 88.196 | 1.00 | 18.43 |
| ATOM | 3780 | N   | ILE | A 476 | 33.889 | 48.860 | 90.723 | 1.00 | 17.01 |
| ATOM | 3781 | CA  | ILE | A 476 | 32.863 | 48.392 | 91.626 | 1.00 | 15.67 |
| ATOM | 3782 | C   | ILE | A 476 | 33.337 | 48.303 | 93.073 | 1.00 | 22.88 |
| ATOM | 3783 | O   | ILE | A 476 | 32.560 | 48.507 | 93.997 | 1.00 | 23.93 |
| ATOM | 3784 | CB  | ILE | A 476 | 32.381 | 47.041 | 91.149 | 1.00 | 18.98 |
| ATOM | 3785 | CG1 | ILE | A 476 | 31.745 | 47.155 | 89.782 | 1.00 | 17.00 |
| ATOM | 3786 | CG2 | ILE | A 476 | 31.515 | 46.303 | 92.172 | 1.00 | 21.59 |
| ATOM | 3787 | CD1 | ILE | A 476 | 31.593 | 45.758 | 89.182 | 1.00 | 22.51 |
| ATOM | 3788 | N   | THR | A 477 | 34.607 | 47.988 | 93.292 | 1.00 | 20.07 |
| ATOM | 3789 | CA  | THR | A 477 | 35.098 | 47.868 | 94.662 | 1.00 | 20.33 |
| ATOM | 3790 | C   | THR | A 477 | 35.996 | 49.039 | 95.113 | 1.00 | 23.48 |
| ATOM | 3791 | O   | THR | A 477 | 36.579 | 49.045 | 96.212 | 1.00 | 21.35 |
| ATOM | 3792 | CB  | THR | A 477 | 35.903 | 46.567 | 94.760 | 1.00 | 26.57 |
| ATOM | 3793 | OG1 | THR | A 477 | 37.068 | 46.687 | 93.950 | 1.00 | 23.03 |
| ATOM | 3794 | CG2 | THR | A 477 | 35.062 | 45.398 | 94.257 | 1.00 | 22.91 |
| ATOM | 3795 | N   | ALA | A 478 | 36.132 | 50.070 | 94.266 | 1.00 | 20.12 |
| ATOM | 3796 | CA  | ALA | A 478 | 37.000 | 51.208 | 94.577 | 1.00 | 16.11 |
| ATOM | 3797 | C   | ALA | A 478 | 36.640 | 51.925 | 95.852 | 1.00 | 23.32 |
| ATOM | 3798 | O   | ALA | A 478 | 35.485 | 52.053 | 96.215 | 1.00 | 24.79 |



00422410 022699

|      |      |     |     |       |        |        |         |      |        |
|------|------|-----|-----|-------|--------|--------|---------|------|--------|
| ATOM | 3799 | CB  | ALA | A 478 | 36.947 | 52.231 | 93.452  | 1.00 | 16.80  |
| ATOM | 3800 | N   | LYS | A 479 | 37.643 | 52.453 | 96.506  | 1.00 | 20.79  |
| ATOM | 3801 | CA  | LYS | A 479 | 37.431 | 53.214 | 97.710  | 1.00 | 19.91  |
| ATOM | 3802 | C   | LYS | A 479 | 38.062 | 54.584 | 97.475  | 1.00 | 24.93  |
| ATOM | 3803 | O   | LYS | A 479 | 38.666 | 54.815 | 96.421  | 1.00 | 21.31  |
| ATOM | 3804 | CB  | LYS | A 479 | 38.008 | 52.527 | 98.946  | 1.00 | 21.40  |
| ATOM | 3805 | CG  | LYS | A 479 | 37.277 | 51.235 | 99.269  | 1.00 | 30.67  |
| ATOM | 3806 | CD  | LYS | A 479 | 37.479 | 50.754 | 100.695 | 1.00 | 26.84  |
| ATOM | 3807 | CE  | LYS | A 479 | 36.139 | 50.430 | 101.349 | 1.00 | 61.23  |
| ATOM | 3808 | NZ  | LYS | A 479 | 35.893 | 48.993 | 101.540 | 1.00 | 56.94  |
| ATOM | 3809 | N   | GLU | A 480 | 37.915 | 55.478 | 98.461  | 1.00 | 20.21  |
| ATOM | 3810 | CA  | GLU | A 480 | 38.458 | 56.794 | 98.368  | 1.00 | 19.79  |
| ATOM | 3811 | C   | GLU | A 480 | 39.871 | 56.781 | 97.857  | 1.00 | 24.31  |
| ATOM | 3812 | O   | GLU | A 480 | 40.211 | 57.522 | 96.942  | 1.00 | 24.33  |
| ATOM | 3813 | CB  | GLU | A 480 | 38.450 | 57.539 | 99.736  | 1.00 | 23.77  |
| ATOM | 3814 | CG  | GLU | A 480 | 39.587 | 58.602 | 99.845  | 1.00 | 50.65  |
| ATOM | 3815 | CD  | GLU | A 480 | 40.676 | 58.361 | 100.891 | 1.00 | 92.31  |
| ATOM | 3816 | OE1 | GLU | A 480 | 40.466 | 57.914 | 102.018 | 1.00 | 100.00 |
| ATOM | 3817 | OE2 | GLU | A 480 | 41.876 | 58.721 | 100.467 | 1.00 | 61.00  |
| ATOM | 3818 | N   | ASP | A 481 | 40.719 | 55.978 | 98.463  | 1.00 | 18.88  |
| ATOM | 3819 | CA  | ASP | A 481 | 42.108 | 55.960 | 98.058  | 1.00 | 20.42  |
| ATOM | 3820 | C   | ASP | A 481 | 42.402 | 55.419 | 96.666  | 1.00 | 24.75  |
| ATOM | 3821 | O   | ASP | A 481 | 43.568 | 55.429 | 96.273  | 1.00 | 24.36  |
| ATOM | 3822 | CB  | ASP | A 481 | 43.028 | 55.281 | 99.094  | 1.00 | 24.59  |
| ATOM | 3823 | CG  | ASP | A 481 | 42.801 | 53.787 | 99.146  | 1.00 | 32.90  |
| ATOM | 3824 | OD1 | ASP | A 481 | 42.001 | 53.254 | 98.393  | 1.00 | 25.09  |
| ATOM | 3825 | OD2 | ASP | A 481 | 43.502 | 53.151 | 100.099 | 1.00 | 15.96  |
| ATOM | 3826 | N   | ASP | A 482 | 41.403 | 54.934 | 95.911  | 1.00 | 20.60  |
| ATOM | 3827 | CA  | ASP | A 482 | 41.682 | 54.431 | 94.553  | 1.00 | 17.36  |
| ATOM | 3828 | C   | ASP | A 482 | 41.291 | 55.406 | 93.452  | 1.00 | 23.26  |
| ATOM | 3829 | O   | ASP | A 482 | 41.684 | 55.278 | 92.300  | 1.00 | 22.77  |
| ATOM | 3830 | CB  | ASP | A 482 | 40.957 | 53.088 | 94.261  | 1.00 | 19.83  |
| ATOM | 3831 | CG  | ASP | A 482 | 41.251 | 52.049 | 95.322  | 1.00 | 21.84  |
| ATOM | 3832 | OD1 | ASP | A 482 | 42.350 | 51.577 | 95.508  | 1.00 | 26.18  |
| ATOM | 3833 | OD2 | ASP | A 482 | 40.212 | 51.759 | 96.060  | 1.00 | 24.50  |
| ATOM | 3834 | N   | LEU | A 483 | 40.479 | 56.384 | 93.785  | 1.00 | 19.29  |
| ATOM | 3835 | CA  | LEU | A 483 | 39.994 | 57.287 | 92.761  | 1.00 | 19.61  |
| ATOM | 3836 | C   | LEU | A 483 | 41.047 | 58.011 | 91.918  | 1.00 | 28.05  |
| ATOM | 3837 | O   | LEU | A 483 | 40.892 | 58.164 | 90.689  | 1.00 | 23.72  |
| ATOM | 3838 | CB  | LEU | A 483 | 38.983 | 58.255 | 93.385  | 1.00 | 18.83  |
| ATOM | 3839 | CG  | LEU | A 483 | 37.801 | 57.488 | 93.925  | 1.00 | 21.23  |
| ATOM | 3840 | CD1 | LEU | A 483 | 36.843 | 58.474 | 94.558  | 1.00 | 22.21  |
| ATOM | 3841 | CD2 | LEU | A 483 | 37.102 | 56.761 | 92.775  | 1.00 | 21.62  |
| ATOM | 3842 | N   | ASN | A 484 | 42.109 | 58.476 | 92.604  | 1.00 | 24.68  |
| ATOM | 3843 | CA  | ASN | A 484 | 43.184 | 59.241 | 91.977  | 1.00 | 26.32  |
| ATOM | 3844 | C   | ASN | A 484 | 44.011 | 58.460 | 91.037  | 1.00 | 29.70  |
| ATOM | 3845 | O   | ASN | A 484 | 44.687 | 59.004 | 90.187  | 1.00 | 31.57  |
| ATOM | 3846 | CB  | ASN | A 484 | 44.126 | 59.910 | 92.991  | 1.00 | 36.64  |
| ATOM | 3847 | CG  | ASN | A 484 | 43.400 | 60.944 | 93.852  | 1.00 | 100.00 |
| ATOM | 3848 | OD1 | ASN | A 484 | 42.425 | 61.578 | 93.405  | 1.00 | 100.00 |
| ATOM | 3849 | ND2 | ASN | A 484 | 43.857 | 61.118 | 95.095  | 1.00 | 100.00 |
| ATOM | 3850 | N   | SER | A 485 | 43.975 | 57.186 | 91.187  | 1.00 | 24.87  |
| ATOM | 3851 | CA  | SER | A 485 | 44.786 | 56.391 | 90.316  | 1.00 | 24.26  |
| ATOM | 3852 | C   | SER | A 485 | 44.060 | 56.018 | 89.023  | 1.00 | 28.05  |
| ATOM | 3853 | O   | SER | A 485 | 44.668 | 55.665 | 88.013  | 1.00 | 28.11  |
| ATOM | 3854 | CB  | SER | A 485 | 45.327 | 55.218 | 91.097  | 1.00 | 29.76  |
| ATOM | 3855 | OG  | SER | A 485 | 46.024 | 55.751 | 92.209  | 1.00 | 46.93  |
| ATOM | 3856 | N   | PHE | A 486 | 42.734 | 56.090 | 89.013  | 1.00 | 20.20  |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 3857 | CA  | PHE | A | 486 | 42.154 | 55.742 | 87.746 | 1.00 | 17.21 |
| ATOM | 3858 | C   | PHE | A | 486 | 42.721 | 56.757 | 86.803 | 1.00 | 18.14 |
| ATOM | 3859 | O   | PHE | A | 486 | 43.058 | 57.852 | 87.215 | 1.00 | 17.89 |
| ATOM | 3860 | CB  | PHE | A | 486 | 40.634 | 55.739 | 87.757 | 1.00 | 18.39 |
| ATOM | 3861 | CG  | PHE | A | 486 | 40.103 | 54.583 | 88.557 | 1.00 | 16.02 |
| ATOM | 3862 | CD1 | PHE | A | 486 | 40.200 | 53.282 | 88.075 | 1.00 | 16.61 |
| ATOM | 3863 | CD2 | PHE | A | 486 | 39.465 | 54.795 | 89.773 | 1.00 | 18.83 |
| ATOM | 3864 | CE1 | PHE | A | 486 | 39.690 | 52.209 | 88.803 | 1.00 | 18.00 |
| ATOM | 3865 | CE2 | PHE | A | 486 | 38.945 | 53.737 | 90.521 | 1.00 | 19.85 |
| ATOM | 3866 | CZ  | PHE | A | 486 | 39.061 | 52.441 | 90.026 | 1.00 | 18.48 |
| ATOM | 3867 | N   | ASN | A | 487 | 42.861 | 56.383 | 85.562 | 1.00 | 21.79 |
| ATOM | 3868 | CA  | ASN | A | 487 | 43.441 | 57.269 | 84.603 | 1.00 | 23.98 |
| ATOM | 3869 | C   | ASN | A | 487 | 43.040 | 56.857 | 83.218 | 1.00 | 25.59 |
| ATOM | 3870 | O   | ASN | A | 487 | 42.702 | 55.697 | 82.974 | 1.00 | 25.22 |
| ATOM | 3871 | CB  | ASN | A | 487 | 44.971 | 57.094 | 84.710 | 1.00 | 27.75 |
| ATOM | 3872 | CG  | ASN | A | 487 | 45.738 | 58.097 | 83.882 | 1.00 | 47.24 |
| ATOM | 3873 | OD1 | ASN | A | 487 | 45.861 | 57.971 | 82.652 | 1.00 | 29.73 |
| ATOM | 3874 | ND2 | ASN | A | 487 | 46.225 | 59.124 | 84.561 | 1.00 | 45.44 |
| ATOM | 3875 | N   | ALA | A | 488 | 43.112 | 57.831 | 82.323 | 1.00 | 24.55 |
| ATOM | 3876 | CA  | ALA | A | 488 | 42.772 | 57.622 | 80.931 | 1.00 | 27.10 |
| ATOM | 3877 | C   | ALA | A | 488 | 43.584 | 56.498 | 80.330 | 1.00 | 31.70 |
| ATOM | 3878 | O   | ALA | A | 488 | 43.193 | 55.858 | 79.348 | 1.00 | 34.84 |
| ATOM | 3879 | CB  | ALA | A | 488 | 42.935 | 58.913 | 80.151 | 1.00 | 29.22 |
| ATOM | 3880 | N   | THR | A | 489 | 44.724 | 56.236 | 80.941 | 1.00 | 29.49 |
| ATOM | 3881 | CA  | THR | A | 489 | 45.561 | 55.162 | 80.435 | 1.00 | 30.81 |
| ATOM | 3882 | C   | THR | A | 489 | 44.925 | 53.824 | 80.631 | 1.00 | 30.86 |
| ATOM | 3883 | O   | THR | A | 489 | 45.323 | 52.852 | 80.020 | 1.00 | 30.02 |
| ATOM | 3884 | CB  | THR | A | 489 | 46.976 | 55.160 | 81.011 | 1.00 | 38.41 |
| ATOM | 3885 | OG1 | THR | A | 489 | 46.912 | 55.010 | 82.404 | 1.00 | 41.46 |
| ATOM | 3886 | CG2 | THR | A | 489 | 47.637 | 56.480 | 80.660 | 1.00 | 38.83 |
| ATOM | 3887 | N   | ASP | A | 490 | 43.929 | 53.794 | 81.490 | 1.00 | 24.45 |
| ATOM | 3888 | CA  | ASP | A | 490 | 43.233 | 52.543 | 81.746 | 1.00 | 24.97 |
| ATOM | 3889 | C   | ASP | A | 490 | 42.601 | 51.948 | 80.493 | 1.00 | 22.10 |
| ATOM | 3890 | O   | ASP | A | 490 | 42.425 | 50.748 | 80.402 | 1.00 | 22.01 |
| ATOM | 3891 | CB  | ASP | A | 490 | 42.088 | 52.721 | 82.799 | 1.00 | 25.90 |
| ATOM | 3892 | CG  | ASP | A | 490 | 42.562 | 53.055 | 84.171 | 1.00 | 24.88 |
| ATOM | 3893 | OD1 | ASP | A | 490 | 43.680 | 52.794 | 84.564 | 1.00 | 25.35 |
| ATOM | 3894 | OD2 | ASP | A | 490 | 41.658 | 53.659 | 84.887 | 1.00 | 19.90 |
| ATOM | 3895 | N   | LEU | A | 491 | 42.204 | 52.815 | 79.565 | 1.00 | 21.62 |
| ATOM | 3896 | CA  | LEU | A | 491 | 41.511 | 52.435 | 78.358 | 1.00 | 20.35 |
| ATOM | 3897 | C   | LEU | A | 491 | 42.419 | 52.134 | 77.204 | 1.00 | 24.60 |
| ATOM | 3898 | O   | LEU | A | 491 | 41.953 | 51.804 | 76.129 | 1.00 | 22.93 |
| ATOM | 3899 | CB  | LEU | A | 491 | 40.558 | 53.558 |        |      |       |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 3915 | O   | ASP | A | 493 | 42.920 | 47.035 | 74.328 | 1.00 | 39.47 |
| ATOM | 3916 | CB  | ASP | A | 493 | 45.457 | 47.814 | 75.017 | 1.00 | 37.95 |
| ATOM | 3917 | CG  | ASP | A | 493 | 46.796 | 48.476 | 75.218 | 1.00 | 55.04 |
| ATOM | 3918 | OD1 | ASP | A | 493 | 47.339 | 49.149 | 74.345 | 1.00 | 60.98 |
| ATOM | 3919 | OD2 | ASP | A | 493 | 47.283 | 48.292 | 76.433 | 1.00 | 44.86 |
| ATOM | 3920 | N   | LEU | A | 494 | 41.953 | 48.969 | 75.054 | 1.00 | 27.85 |
| ATOM | 3921 | CA  | LEU | A | 494 | 40.598 | 48.497 | 75.031 | 1.00 | 23.42 |
| ATOM | 3922 | C   | LEU | A | 494 | 39.891 | 48.937 | 73.771 | 1.00 | 26.34 |
| ATOM | 3923 | O   | LEU | A | 494 | 39.878 | 50.114 | 73.446 | 1.00 | 28.45 |
| ATOM | 3924 | CB  | LEU | A | 494 | 39.835 | 49.057 | 76.234 | 1.00 | 21.52 |
| ATOM | 3925 | CG  | LEU | A | 494 | 40.341 | 48.550 | 77.564 | 1.00 | 21.47 |
| ATOM | 3926 | CD1 | LEU | A | 494 | 39.298 | 48.922 | 78.586 | 1.00 | 21.58 |
| ATOM | 3927 | CD2 | LEU | A | 494 | 40.490 | 47.032 | 77.551 | 1.00 | 22.77 |
| ATOM | 3928 | N   | SER | A | 495 | 39.288 | 47.978 | 73.065 | 1.00 | 18.61 |
| ATOM | 3929 | CA  | SER | A | 495 | 38.543 | 48.304 | 71.882 | 1.00 | 18.82 |
| ATOM | 3930 | C   | SER | A | 495 | 37.207 | 48.925 | 72.308 | 1.00 | 22.38 |
| ATOM | 3931 | O   | SER | A | 495 | 36.791 | 48.850 | 73.479 | 1.00 | 18.55 |
| ATOM | 3932 | CB  | SER | A | 495 | 38.244 | 47.030 | 71.131 | 1.00 | 20.60 |
| ATOM | 3933 | OG  | SER | A | 495 | 37.346 | 46.263 | 71.937 | 1.00 | 24.08 |
| ATOM | 3934 | N   | SER | A | 496 | 36.513 | 49.517 | 71.355 | 1.00 | 19.51 |
| ATOM | 3935 | CA  | SER | A | 496 | 35.232 | 50.083 | 71.680 | 1.00 | 19.05 |
| ATOM | 3936 | C   | SER | A | 496 | 34.360 | 48.953 | 72.243 | 1.00 | 22.03 |
| ATOM | 3937 | O   | SER | A | 496 | 33.577 | 49.165 | 73.174 | 1.00 | 19.08 |
| ATOM | 3938 | CB  | SER | A | 496 | 34.604 | 50.750 | 70.470 | 1.00 | 20.48 |
| ATOM | 3939 | OG  | SER | A | 496 | 34.129 | 49.722 | 69.664 | 1.00 | 27.30 |
| ATOM | 3940 | N   | HIS | A | 497 | 34.539 | 47.730 | 71.700 | 1.00 | 18.16 |
| ATOM | 3941 | CA  | HIS | A | 497 | 33.804 | 46.555 | 72.180 | 1.00 | 18.79 |
| ATOM | 3942 | C   | HIS | A | 497 | 34.034 | 46.302 | 73.674 | 1.00 | 21.10 |
| ATOM | 3943 | O   | HIS | A | 497 | 33.119 | 45.976 | 74.445 | 1.00 | 20.24 |
| ATOM | 3944 | CB  | HIS | A | 497 | 34.159 | 45.285 | 71.362 | 1.00 | 20.44 |
| ATOM | 3945 | CG  | HIS | A | 497 | 33.757 | 45.504 | 69.949 | 1.00 | 28.33 |
| ATOM | 3946 | ND1 | HIS | A | 497 | 34.663 | 45.976 | 68.994 | 1.00 | 33.99 |
| ATOM | 3947 | CD2 | HIS | A | 497 | 32.527 | 45.413 | 69.366 | 1.00 | 31.27 |
| ATOM | 3948 | CE1 | HIS | A | 497 | 33.977 | 46.117 | 67.860 | 1.00 | 33.65 |
| ATOM | 3949 | NE2 | HIS | A | 497 | 32.690 | 45.785 | 68.060 | 1.00 | 33.66 |
| ATOM | 3950 | N   | GLN | A | 498 | 35.281 | 46.439 | 74.074 | 1.00 | 18.94 |
| ATOM | 3951 | CA  | GLN | A | 498 | 35.663 | 46.218 | 75.458 | 1.00 | 17.24 |
| ATOM | 3952 | C   | GLN | A | 498 | 35.169 | 47.290 | 76.384 | 1.00 | 19.29 |
| ATOM | 3953 | O   | GLN | A | 498 | 34.800 | 46.987 | 77.507 | 1.00 | 16.53 |
| ATOM | 3954 | CB  | GLN | A | 498 | 37.149 | 45.987 | 75.601 | 1.00 | 17.60 |
| ATOM | 3955 | CG  | GLN | A | 498 | 37.537 | 44.613 | 75.002 | 1.00 | 21.50 |
| ATOM | 3956 | CD  | GLN | A | 498 | 39.031 | 44.468 | 74.905 | 1.00 | 24.22 |
| ATOM | 3957 | OE1 | GLN | A | 498 | 39.659 | 45.268 | 74.241 | 1.00 | 19.69 |
| ATOM | 3958 | NE2 | GLN | A | 498 | 39.597 | 43.501 | 75.602 | 1.00 | 20.25 |
| ATOM | 3959 | N   | LEU | A | 499 | 35.129 | 48.539 | 75.916 | 1.00 | 20.34 |
| ATOM | 3960 | CA  | LEU | A | 499 | 34.609 | 49.657 | 76.736 | 1.00 | 20.43 |
| ATOM | 3961 | C   | LEU | A | 499 | 33.127 | 49.402 | 77.084 | 1.00 | 20.53 |
| ATOM | 3962 | O   | LEU | A | 499 | 32.638 | 49.601 | 78.228 | 1.00 | 18.25 |
| ATOM | 3963 | CB  | LEU | A | 499 | 34.620 | 50.962 | 75.921 | 1.00 | 21.15 |
| ATOM | 3964 | CG  | LEU | A | 499 | 36.002 | 51.503 | 75.675 | 1.00 | 26.16 |
| ATOM | 3965 | CD1 | LEU | A | 499 | 35.875 | 52.920 | 75.099 | 1.00 | 27.09 |
| ATOM | 3966 | CD2 | LEU | A | 499 | 36.728 | 51.545 | 77.002 | 1.00 | 27.76 |
| ATOM | 3967 | N   | ASN | A | 500 | 32.410 | 48.936 | 76.038 | 1.00 | 16.19 |
| ATOM | 3968 | CA  | ASN | A | 500 | 31.009 | 48.628 | 76.174 | 1.00 | 14.95 |
| ATOM | 3969 | C   | ASN | A | 500 | 30.755 | 47.507 | 77.191 | 1.00 | 15.08 |
| ATOM | 3970 | O   | ASN | A | 500 | 29.853 | 47.590 | 78.034 | 1.00 | 16.94 |
| ATOM | 3971 | CB  | ASN | A | 500 | 30.430 | 48.314 | 74.794 | 1.00 | 16.19 |
| ATOM | 3972 | CG  | ASN | A | 500 | 28.938 | 48.113 | 74.817 | 1.00 | 26.36 |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 3973 | OD1 | ASN | A | 500 | 28.161 | 48.965 | 75.284 | 1.00 | 26.44 |
| ATOM | 3974 | ND2 | ASN | A | 500 | 28.532 | 46.966 | 74.321 | 1.00 | 28.52 |
| ATOM | 3975 | N   | GLU | A | 501 | 31.558 | 46.458 | 77.099 | 1.00 | 11.19 |
| ATOM | 3976 | CA  | GLU | A | 501 | 31.426 | 45.333 | 78.006 | 1.00 | 13.12 |
| ATOM | 3977 | C   | GLU | A | 501 | 31.768 | 45.748 | 79.427 | 1.00 | 15.66 |
| ATOM | 3978 | O   | GLU | A | 501 | 31.172 | 45.299 | 80.401 | 1.00 | 15.79 |
| ATOM | 3979 | CB  | GLU | A | 501 | 32.343 | 44.197 | 77.600 | 1.00 | 16.26 |
| ATOM | 3980 | CG  | GLU | A | 501 | 32.213 | 43.004 | 78.571 | 1.00 | 18.32 |
| ATOM | 3981 | CD  | GLU | A | 501 | 30.807 | 42.412 | 78.640 | 1.00 | 45.05 |
| ATOM | 3982 | OE1 | GLU | A | 501 | 29.953 | 42.623 | 77.802 | 1.00 | 25.19 |
| ATOM | 3983 | OE2 | GLU | A | 501 | 30.582 | 41.647 | 79.694 | 1.00 | 28.99 |
| ATOM | 3984 | N   | PHE | A | 502 | 32.758 | 46.625 | 79.528 | 1.00 | 13.04 |
| ATOM | 3985 | CA  | PHE | A | 502 | 33.195 | 47.161 | 80.792 | 1.00 | 14.85 |
| ATOM | 3986 | C   | PHE | A | 502 | 32.009 | 47.853 | 81.479 | 1.00 | 16.26 |
| ATOM | 3987 | O   | PHE | A | 502 | 31.683 | 47.658 | 82.653 | 1.00 | 14.73 |
| ATOM | 3988 | CB  | PHE | A | 502 | 34.343 | 48.173 | 80.519 | 1.00 | 17.18 |
| ATOM | 3989 | CG  | PHE | A | 502 | 34.522 | 49.209 | 81.611 | 1.00 | 17.10 |
| ATOM | 3990 | CD1 | PHE | A | 502 | 34.862 | 48.837 | 82.909 | 1.00 | 16.09 |
| ATOM | 3991 | CD2 | PHE | A | 502 | 34.343 | 50.566 | 81.340 | 1.00 | 19.32 |
| ATOM | 3992 | CE1 | PHE | A | 502 | 35.023 | 49.787 | 83.920 | 1.00 | 19.64 |
| ATOM | 3993 | CE2 | PHE | A | 502 | 34.482 | 51.528 | 82.338 | 1.00 | 21.09 |
| ATOM | 3994 | CZ  | PHE | A | 502 | 34.826 | 51.142 | 83.632 | 1.00 | 20.37 |
| ATOM | 3995 | N   | LEU | A | 503 | 31.371 | 48.676 | 80.686 | 1.00 | 13.41 |
| ATOM | 3996 | CA  | LEU | A | 503 | 30.240 | 49.412 | 81.162 | 1.00 | 14.23 |
| ATOM | 3997 | C   | LEU | A | 503 | 29.077 | 48.486 | 81.516 | 1.00 | 17.32 |
| ATOM | 3998 | O   | LEU | A | 503 | 28.386 | 48.671 | 82.526 | 1.00 | 16.59 |
| ATOM | 3999 | CB  | LEU | A | 503 | 29.807 | 50.457 | 80.105 | 1.00 | 14.70 |
| ATOM | 4000 | CG  | LEU | A | 503 | 30.726 | 51.674 | 80.068 | 1.00 | 17.55 |
| ATOM | 4001 | CD1 | LEU | A | 503 | 30.419 | 52.538 | 78.859 | 1.00 | 14.03 |
| ATOM | 4002 | CD2 | LEU | A | 503 | 30.471 | 52.511 | 81.298 | 1.00 | 16.66 |
| ATOM | 4003 | N   | ALA | A | 504 | 28.850 | 47.485 | 80.656 | 1.00 | 13.74 |
| ATOM | 4004 | CA  | ALA | A | 504 | 27.773 | 46.557 | 80.894 | 1.00 | 12.59 |
| ATOM | 4005 | C   | ALA | A | 504 | 27.999 | 45.866 | 82.222 | 1.00 | 16.53 |
| ATOM | 4006 | O   | ALA | A | 504 | 27.098 | 45.679 | 83.043 | 1.00 | 14.36 |
| ATOM | 4007 | CB  | ALA | A | 504 | 27.728 | 45.522 | 79.764 | 1.00 | 12.80 |
| ATOM | 4008 | N   | GLN | A | 505 | 29.248 | 45.463 | 82.436 | 1.00 | 15.92 |
| ATOM | 4009 | CA  | GLN | A | 505 | 29.522 | 44.794 | 83.682 | 1.00 | 16.60 |
| ATOM | 4010 | C   | GLN | A | 505 | 29.325 | 45.750 | 84.852 | 1.00 | 20.60 |
| ATOM | 4011 | O   | GLN | A | 505 | 28.804 | 45.372 | 85.908 | 1.00 | 19.55 |
| ATOM | 4012 | CB  | GLN | A | 505 | 30.918 | 44.175 | 83.723 | 1.00 | 17.18 |
| ATOM | 4013 | CG  | GLN | A | 505 | 31.138 | 43.133 | 82.613 | 1.00 | 19.88 |
| ATOM | 4014 | CD  | GLN | A | 505 | 32.590 | 42.647 | 82.571 | 1.00 | 41.41 |
| ATOM | 4015 | OE1 | GLN | A | 505 |        |        |        |      |       |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 4031 | CD2 | LEU | A | 507 | 23.610 | 49.318 | 82.335 | 1.00 | 22.64 |
| ATOM | 4032 | N   | GLN | A | 508 | 25.686 | 46.285 | 85.754 | 1.00 | 18.81 |
| ATOM | 4033 | CA  | GLN | A | 508 | 25.036 | 45.213 | 86.478 | 1.00 | 17.54 |
| ATOM | 4034 | C   | GLN | A | 508 | 25.141 | 45.432 | 88.007 | 1.00 | 24.09 |
| ATOM | 4035 | O   | GLN | A | 508 | 24.382 | 44.861 | 88.816 | 1.00 | 23.10 |
| ATOM | 4036 | CB  | GLN | A | 508 | 25.655 | 43.859 | 86.136 | 1.00 | 17.62 |
| ATOM | 4037 | CG  | GLN | A | 508 | 25.383 | 43.365 | 84.699 | 1.00 | 35.49 |
| ATOM | 4038 | CD  | GLN | A | 508 | 25.734 | 41.880 | 84.540 | 1.00 | 39.81 |
| ATOM | 4039 | OE1 | GLN | A | 508 | 26.759 | 41.440 | 85.074 | 1.00 | 23.94 |
| ATOM | 4040 | NE2 | GLN | A | 508 | 24.870 | 41.090 | 83.871 | 1.00 | 20.37 |
| ATOM | 4041 | N   | ARG | A | 509 | 26.085 | 46.268 | 88.430 | 1.00 | 19.00 |
| ATOM | 4042 | CA  | ARG | A | 509 | 26.279 | 46.528 | 89.849 | 1.00 | 19.42 |
| ATOM | 4043 | C   | ARG | A | 509 | 25.878 | 47.952 | 90.230 | 1.00 | 25.44 |
| ATOM | 4044 | O   | ARG | A | 509 | 26.207 | 48.445 | 91.317 | 1.00 | 27.11 |
| ATOM | 4045 | CB  | ARG | A | 509 | 27.696 | 46.182 | 90.352 | 1.00 | 20.80 |
| ATOM | 4046 | CG  | ARG | A | 509 | 28.145 | 44.770 | 89.965 | 1.00 | 28.27 |
| ATOM | 4047 | CD  | ARG | A | 509 | 27.749 | 43.726 | 90.993 | 1.00 | 46.76 |
| ATOM | 4048 | NE  | ARG | A | 509 | 28.476 | 43.944 | 92.247 | 1.00 | 78.35 |
| ATOM | 4049 | CZ  | ARG | A | 509 | 29.639 | 43.368 | 92.585 | 1.00 | 79.72 |
| ATOM | 4050 | NH1 | ARG | A | 509 | 30.276 | 42.489 | 91.795 | 1.00 | 53.80 |
| ATOM | 4051 | NH2 | ARG | A | 509 | 30.169 | 43.687 | 93.762 | 1.00 | 60.24 |
| ATOM | 4052 | N   | ALA | A | 510 | 25.155 | 48.625 | 89.337 | 1.00 | 20.12 |
| ATOM | 4053 | CA  | ALA | A | 510 | 24.752 | 49.967 | 89.669 | 1.00 | 18.42 |
| ATOM | 4054 | C   | ALA | A | 510 | 23.784 | 49.926 | 90.838 | 1.00 | 25.78 |
| ATOM | 4055 | O   | ALA | A | 510 | 23.077 | 48.939 | 91.025 | 1.00 | 23.74 |
| ATOM | 4056 | CB  | ALA | A | 510 | 24.145 | 50.643 | 88.477 | 1.00 | 17.78 |
| ATOM | 4057 | N   | PRO | A | 511 | 23.759 | 50.985 | 91.650 | 1.00 | 25.50 |
| ATOM | 4058 | CA  | PRO | A | 511 | 24.544 | 52.194 | 91.447 | 1.00 | 23.03 |
| ATOM | 4059 | C   | PRO | A | 511 | 25.898 | 52.188 | 92.076 | 1.00 | 23.95 |
| ATOM | 4060 | O   | PRO | A | 511 | 26.156 | 51.518 | 93.052 | 1.00 | 22.19 |
| ATOM | 4061 | CB  | PRO | A | 511 | 23.824 | 53.261 | 92.253 | 1.00 | 22.56 |
| ATOM | 4062 | CG  | PRO | A | 511 | 23.137 | 52.505 | 93.370 | 1.00 | 29.69 |
| ATOM | 4063 | CD  | PRO | A | 511 | 22.975 | 51.070 | 92.900 | 1.00 | 26.79 |
| ATOM | 4064 | N   | LEU | A | 512 | 26.732 | 53.019 | 91.512 | 1.00 | 20.39 |
| ATOM | 4065 | CA  | LEU | A | 512 | 28.028 | 53.234 | 92.046 | 1.00 | 21.08 |
| ATOM | 4066 | C   | LEU | A | 512 | 27.901 | 54.569 | 92.773 | 1.00 | 24.40 |
| ATOM | 4067 | O   | LEU | A | 512 | 26.977 | 55.361 | 92.485 | 1.00 | 22.11 |
| ATOM | 4068 | CB  | LEU | A | 512 | 29.056 | 53.362 | 90.914 | 1.00 | 23.71 |
| ATOM | 4069 | CG  | LEU | A | 512 | 29.726 | 52.029 | 90.535 | 1.00 | 29.56 |
| ATOM | 4070 | CD1 | LEU | A | 512 | 28.684 | 50.974 | 90.097 | 1.00 | 29.29 |
| ATOM | 4071 | CD2 | LEU | A | 512 | 30.679 | 52.329 | 89.388 | 1.00 | 35.20 |
| ATOM | 4072 | N   | PRO | A | 513 | 28.795 | 54.837 | 93.722 | 1.00 | 20.62 |
| ATOM | 4073 | CA  | PRO | A | 513 | 28.697 |        |        |      |       |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 4089 | C   | GLY | A | 515 | 32.448 | 59.638 | 92.469 | 1.00 | 23.12 |
| ATOM | 4090 | O   | GLY | A | 515 | 33.286 | 60.105 | 91.687 | 1.00 | 23.24 |
| ATOM | 4091 | N   | HIS | A | 516 | 32.150 | 58.337 | 92.477 | 1.00 | 19.26 |
| ATOM | 4092 | CA  | HIS | A | 516 | 32.835 | 57.435 | 91.550 | 1.00 | 18.68 |
| ATOM | 4093 | C   | HIS | A | 516 | 32.466 | 57.705 | 90.105 | 1.00 | 17.66 |
| ATOM | 4094 | O   | HIS | A | 516 | 33.295 | 57.751 | 89.221 | 1.00 | 17.29 |
| ATOM | 4095 | CB  | HIS | A | 516 | 32.617 | 55.957 | 91.861 | 1.00 | 18.09 |
| ATOM | 4096 | CG  | HIS | A | 516 | 33.216 | 55.585 | 93.169 | 1.00 | 23.48 |
| ATOM | 4097 | ND1 | HIS | A | 516 | 33.588 | 54.271 | 93.463 | 1.00 | 27.23 |
| ATOM | 4098 | CD2 | HIS | A | 516 | 33.486 | 56.344 | 94.256 | 1.00 | 26.54 |
| ATOM | 4099 | CE1 | HIS | A | 516 | 34.072 | 54.256 | 94.699 | 1.00 | 25.60 |
| ATOM | 4100 | NE2 | HIS | A | 516 | 34.028 | 55.481 | 95.205 | 1.00 | 27.20 |
| ATOM | 4101 | N   | ILE | A | 517 | 31.198 | 57.925 | 89.871 | 1.00 | 15.26 |
| ATOM | 4102 | CA  | ILE | A | 517 | 30.787 | 58.158 | 88.523 | 1.00 | 16.45 |
| ATOM | 4103 | C   | ILE | A | 517 | 31.347 | 59.465 | 88.034 | 1.00 | 17.88 |
| ATOM | 4104 | O   | ILE | A | 517 | 31.807 | 59.622 | 86.910 | 1.00 | 17.44 |
| ATOM | 4105 | CB  | ILE | A | 517 | 29.274 | 58.016 | 88.371 | 1.00 | 23.63 |
| ATOM | 4106 | CG1 | ILE | A | 517 | 28.826 | 56.606 | 88.810 | 1.00 | 25.40 |
| ATOM | 4107 | CG2 | ILE | A | 517 | 28.830 | 58.270 | 86.925 | 1.00 | 26.36 |
| ATOM | 4108 | CD1 | ILE | A | 517 | 29.394 | 55.444 | 87.985 | 1.00 | 22.65 |
| ATOM | 4109 | N   | LYS | A | 518 | 31.344 | 60.426 | 88.912 | 1.00 | 16.53 |
| ATOM | 4110 | CA  | LYS | A | 518 | 31.906 | 61.699 | 88.505 | 1.00 | 17.58 |
| ATOM | 4111 | C   | LYS | A | 518 | 33.372 | 61.521 | 88.084 | 1.00 | 20.03 |
| ATOM | 4112 | O   | LYS | A | 518 | 33.826 | 62.082 | 87.101 | 1.00 | 16.13 |
| ATOM | 4113 | CB  | LYS | A | 518 | 31.770 | 62.744 | 89.631 | 1.00 | 15.25 |
| ATOM | 4114 | CG  | LYS | A | 518 | 30.350 | 63.266 | 89.751 | 1.00 | 14.67 |
| ATOM | 4115 | CD  | LYS | A | 518 | 30.170 | 64.148 | 90.965 | 1.00 | 20.03 |
| ATOM | 4116 | CE  | LYS | A | 518 | 28.844 | 64.880 | 90.939 | 1.00 | 32.46 |
| ATOM | 4117 | NZ  | LYS | A | 518 | 28.728 | 65.790 | 92.088 | 1.00 | 50.93 |
| ATOM | 4118 | N   | ARG | A | 519 | 34.110 | 60.724 | 88.865 | 1.00 | 18.45 |
| ATOM | 4119 | CA  | ARG | A | 519 | 35.512 | 60.472 | 88.617 | 1.00 | 15.13 |
| ATOM | 4120 | C   | ARG | A | 519 | 35.683 | 59.760 | 87.297 | 1.00 | 18.23 |
| ATOM | 4121 | O   | ARG | A | 519 | 36.584 | 60.047 | 86.503 | 1.00 | 17.57 |
| ATOM | 4122 | CB  | ARG | A | 519 | 36.138 | 59.655 | 89.746 | 1.00 | 13.90 |
| ATOM | 4123 | CG  | ARG | A | 519 | 37.604 | 59.313 | 89.444 | 1.00 | 15.17 |
| ATOM | 4124 | CD  | ARG | A | 519 | 38.522 | 60.538 | 89.464 | 1.00 | 25.46 |
| ATOM | 4125 | NE  | ARG | A | 519 | 39.959 | 60.229 | 89.280 | 1.00 | 25.30 |
| ATOM | 4126 | CZ  | ARG | A | 519 | 40.836 | 61.098 | 88.768 | 1.00 | 29.02 |
| ATOM | 4127 | NH1 | ARG | A | 519 | 40.478 | 62.322 | 88.355 | 1.00 | 25.41 |
| ATOM | 4128 | NH2 | ARG | A | 519 | 42.093 | 60.731 | 88.649 | 1.00 | 20.47 |
| ATOM | 4129 | N   | MET | A | 520 | 34.784 | 58.815 | 87.054 | 1.00 | 15.71 |
| ATOM | 4130 | CA  | MET | A | 520 | 34.835 | 58.067 | 85.805 | 1.00 | 13.65 |
| ATOM | 4131 | C   | MET | A | 520 | 34.710 | 59.    |        |      |       |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 4147 | CA  | GLU | A | 522 | 36.821 | 62.966 | 84.706 | 1.00 | 17.15 |
| ATOM | 4148 | C   | GLU | A | 522 | 38.007 | 62.218 | 84.051 | 1.00 | 25.41 |
| ATOM | 4149 | O   | GLU | A | 522 | 38.860 | 62.814 | 83.370 | 1.00 | 20.91 |
| ATOM | 4150 | CB  | GLU | A | 522 | 37.318 | 63.258 | 86.109 | 1.00 | 19.27 |
| ATOM | 4151 | CG  | GLU | A | 522 | 36.560 | 64.272 | 86.977 | 1.00 | 38.73 |
| ATOM | 4152 | CD  | GLU | A | 522 | 37.423 | 64.542 | 88.180 | 1.00 | 59.23 |
| ATOM | 4153 | OE1 | GLU | A | 522 | 38.353 | 65.321 | 88.160 | 1.00 | 77.57 |
| ATOM | 4154 | OE2 | GLU | A | 522 | 37.148 | 63.788 | 89.208 | 1.00 | 62.80 |
| ATOM | 4155 | N   | VAL | A | 523 | 38.120 | 60.903 | 84.278 | 1.00 | 19.75 |
| ATOM | 4156 | CA  | VAL | A | 523 | 39.249 | 60.212 | 83.691 | 1.00 | 16.48 |
| ATOM | 4157 | C   | VAL | A | 523 | 39.045 | 59.583 | 82.320 | 1.00 | 19.65 |
| ATOM | 4158 | O   | VAL | A | 523 | 40.003 | 59.432 | 81.578 | 1.00 | 20.76 |
| ATOM | 4159 | CB  | VAL | A | 523 | 39.870 | 59.234 | 84.668 | 1.00 | 19.84 |
| ATOM | 4160 | CG1 | VAL | A | 523 | 40.209 | 59.969 | 85.953 | 1.00 | 19.70 |
| ATOM | 4161 | CG2 | VAL | A | 523 | 38.892 | 58.115 | 84.997 | 1.00 | 19.64 |
| ATOM | 4162 | N   | TYR | A | 524 | 37.810 | 59.186 | 81.966 | 1.00 | 17.18 |
| ATOM | 4163 | CA  | TYR | A | 524 | 37.566 | 58.516 | 80.679 | 1.00 | 12.15 |
| ATOM | 4164 | C   | TYR | A | 524 | 36.817 | 59.313 | 79.623 | 1.00 | 17.66 |
| ATOM | 4165 | O   | TYR | A | 524 | 36.767 | 58.933 | 78.451 | 1.00 | 16.12 |
| ATOM | 4166 | CB  | TYR | A | 524 | 36.860 | 57.185 | 80.860 | 1.00 | 11.05 |
| ATOM | 4167 | CG  | TYR | A | 524 | 37.563 | 56.240 | 81.797 | 1.00 | 14.57 |
| ATOM | 4168 | CD1 | TYR | A | 524 | 38.948 | 56.199 | 81.935 | 1.00 | 13.44 |
| ATOM | 4169 | CD2 | TYR | A | 524 | 36.784 | 55.367 | 82.556 | 1.00 | 16.79 |
| ATOM | 4170 | CE1 | TYR | A | 524 | 39.530 | 55.296 | 82.832 | 1.00 | 16.24 |
| ATOM | 4171 | CE2 | TYR | A | 524 | 37.354 | 54.455 | 83.443 | 1.00 | 18.03 |
| ATOM | 4172 | CZ  | TYR | A | 524 | 38.739 | 54.419 | 83.580 | 1.00 | 25.46 |
| ATOM | 4173 | OH  | TYR | A | 524 | 39.305 | 53.514 | 84.463 | 1.00 | 20.75 |
| ATOM | 4174 | N   | ASN | A | 525 | 36.209 | 60.400 | 80.039 | 1.00 | 16.08 |
| ATOM | 4175 | CA  | ASN | A | 525 | 35.485 | 61.243 | 79.098 | 1.00 | 16.42 |
| ATOM | 4176 | C   | ASN | A | 525 | 34.439 | 60.482 | 78.253 | 1.00 | 20.20 |
| ATOM | 4177 | O   | ASN | A | 525 | 34.305 | 60.658 | 77.022 | 1.00 | 18.84 |
| ATOM | 4178 | CB  | ASN | A | 525 | 36.460 | 62.041 | 78.243 | 1.00 | 16.14 |
| ATOM | 4179 | CG  | ASN | A | 525 | 35.744 | 63.162 | 77.527 | 1.00 | 23.40 |
| ATOM | 4180 | OD1 | ASN | A | 525 | 34.621 | 63.545 | 77.906 | 1.00 | 17.28 |
| ATOM | 4181 | ND2 | ASN | A | 525 | 36.376 | 63.686 | 76.478 | 1.00 | 18.64 |
| ATOM | 4182 | N   | PHE | A | 526 | 33.653 | 59.641 | 78.949 | 1.00 | 16.41 |
| ATOM | 4183 | CA  | PHE | A | 526 | 32.619 | 58.905 | 78.279 | 1.00 | 15.86 |
| ATOM | 4184 | C   | PHE | A | 526 | 31.540 | 59.825 | 77.704 | 1.00 | 19.88 |
| ATOM | 4185 | O   | PHE | A | 526 | 30.864 | 59.459 | 76.754 | 1.00 | 17.12 |
| ATOM | 4186 | CB  | PHE | A | 526 | 32.011 | 57.849 | 79.207 | 1.00 | 18.58 |
| ATOM | 4187 | CG  | PHE | A | 526 | 32.899 | 56.644 | 79.394 | 1.00 | 21.46 |
| ATOM | 4188 | CD1 | PHE | A | 526 | 33.760 | 56.218 | 78.378 | 1.00 | 26.02 |
| ATOM | 4189 | CD2 | PHE | A | 526 | 32.880 | 55.920 | 80.587 | 1.00 | 21.37 |
| ATOM | 4190 | CE1 | PHE | A | 526 | 34.569 | 55.090 | 78.523 | 1.00 | 24.79 |
| ATOM | 4191 | CE2 | PHE | A | 526 | 33.686 | 54.792 | 80.758 | 1.00 | 21.37 |
| ATOM | 4192 | CZ  | PHE | A | 526 | 34.517 | 54.368 | 79.721 | 1.00 | 20.49 |
| ATOM | 4193 | N   | ASN | A | 527 | 31.322 | 61.012 | 78.276 | 1.00 | 15.47 |
| ATOM | 4194 | CA  | ASN | A | 527 | 30.290 | 61.867 | 77.727 | 1.00 | 13.11 |
| ATOM | 4195 | C   | ASN | A | 527 | 30.607 | 62.185 | 76.300 | 1.00 | 19.43 |
| ATOM | 4196 | O   | ASN | A | 527 | 29.735 | 62.562 | 75.517 | 1.00 | 19.12 |
| ATOM | 4197 | CB  | ASN | A | 527 | 30.211 | 63.232 | 78.409 | 1.00 | 16.84 |
| ATOM | 4198 | CG  | ASN | A | 527 | 29.525 | 63.216 | 79.754 | 1.00 | 27.65 |
| ATOM | 4199 | OD1 | ASN | A | 527 | 29.633 | 64.170 | 80.558 | 1.00 | 22.99 |
| ATOM | 4200 | ND2 | ASN | A | 527 | 28.811 | 62.142 | 80.005 | 1.00 | 12.18 |
| ATOM | 4201 | N   | ALA | A | 528 | 31.886 | 62.083 | 75.972 | 1.00 | 17.86 |
| ATOM | 4202 | CA  | ALA | A | 528 | 32.302 | 62.431 | 74.611 | 1.00 | 19.52 |
| ATOM | 4203 | C   | ALA | A | 528 | 32.076 | 61.351 | 73.550 | 1.00 | 23.88 |
| ATOM | 4204 | O   | ALA | A | 528 | 32.179 | 61.595 | 72.360 | 1.00 | 19.92 |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 4205 | CB  | ALA | A | 528 | 33.777 | 62.815 | 74.605 | 1.00 | 20.88 |
| ATOM | 4206 | N   | ILE | A | 529 | 31.832 | 60.132 | 73.967 | 1.00 | 18.40 |
| ATOM | 4207 | CA  | ILE | A | 529 | 31.678 | 59.056 | 73.009 | 1.00 | 16.46 |
| ATOM | 4208 | C   | ILE | A | 529 | 30.326 | 59.065 | 72.332 | 1.00 | 21.76 |
| ATOM | 4209 | O   | ILE | A | 529 | 29.305 | 59.139 | 72.984 | 1.00 | 22.99 |
| ATOM | 4210 | CB  | ILE | A | 529 | 31.946 | 57.755 | 73.756 | 1.00 | 19.71 |
| ATOM | 4211 | CG1 | ILE | A | 529 | 33.474 | 57.651 | 73.951 | 1.00 | 18.95 |
| ATOM | 4212 | CG2 | ILE | A | 529 | 31.364 | 56.591 | 72.951 | 1.00 | 18.71 |
| ATOM | 4213 | CD1 | ILE | A | 529 | 33.945 | 56.461 | 74.761 | 1.00 | 22.33 |
| ATOM | 4214 | N   | ASN | A | 530 | 30.294 | 58.969 | 71.026 | 1.00 | 22.69 |
| ATOM | 4215 | CA  | ASN | A | 530 | 29.002 | 58.981 | 70.353 | 1.00 | 23.57 |
| ATOM | 4216 | C   | ASN | A | 530 | 28.409 | 57.630 | 69.959 | 1.00 | 26.83 |
| ATOM | 4217 | O   | ASN | A | 530 | 27.248 | 57.564 | 69.552 | 1.00 | 26.76 |
| ATOM | 4218 | CB  | ASN | A | 530 | 28.984 | 59.978 | 69.203 | 1.00 | 38.14 |
| ATOM | 4219 | CG  | ASN | A | 530 | 29.071 | 61.399 | 69.728 | 1.00 | 61.28 |
| ATOM | 4220 | OD1 | ASN | A | 530 | 28.136 | 61.910 | 70.369 | 1.00 | 58.85 |
| ATOM | 4221 | ND2 | ASN | A | 530 | 30.207 | 62.029 | 69.479 | 1.00 | 53.69 |
| ATOM | 4222 | N   | ASN | A | 531 | 29.217 | 56.571 | 70.074 | 1.00 | 21.41 |
| ATOM | 4223 | CA  | ASN | A | 531 | 28.830 | 55.193 | 69.793 | 1.00 | 18.74 |
| ATOM | 4224 | C   | ASN | A | 531 | 27.582 | 54.954 | 70.629 | 1.00 | 20.62 |
| ATOM | 4225 | O   | ASN | A | 531 | 27.591 | 55.148 | 71.848 | 1.00 | 20.50 |
| ATOM | 4226 | CB  | ASN | A | 531 | 29.973 | 54.294 | 70.281 | 1.00 | 19.20 |
| ATOM | 4227 | CG  | ASN | A | 531 | 29.636 | 52.824 | 70.208 | 1.00 | 31.49 |
| ATOM | 4228 | OD1 | ASN | A | 531 | 28.663 | 52.353 | 70.848 | 1.00 | 22.31 |
| ATOM | 4229 | ND2 | ASN | A | 531 | 30.431 | 52.095 | 69.406 | 1.00 | 18.30 |
| ATOM | 4230 | N   | SER | A | 532 | 26.489 | 54.584 | 69.996 | 1.00 | 16.48 |
| ATOM | 4231 | CA  | SER | A | 532 | 25.237 | 54.445 | 70.724 | 1.00 | 16.29 |
| ATOM | 4232 | C   | SER | A | 532 | 25.164 | 53.417 | 71.856 | 1.00 | 18.06 |
| ATOM | 4233 | O   | SER | A | 532 | 24.508 | 53.629 | 72.888 | 1.00 | 20.46 |
| ATOM | 4234 | CB  | SER | A | 532 | 24.032 | 54.424 | 69.782 | 1.00 | 22.96 |
| ATOM | 4235 | OG  | SER | A | 532 | 24.151 | 53.318 | 68.884 | 1.00 | 27.85 |
| ATOM | 4236 | N   | GLU | A | 533 | 25.811 | 52.298 | 71.667 | 1.00 | 12.93 |
| ATOM | 4237 | CA  | GLU | A | 533 | 25.776 | 51.257 | 72.657 | 1.00 | 13.78 |
| ATOM | 4238 | C   | GLU | A | 533 | 26.436 | 51.733 | 73.911 | 1.00 | 22.43 |
| ATOM | 4239 | O   | GLU | A | 533 | 25.912 | 51.551 | 75.031 | 1.00 | 20.25 |
| ATOM | 4240 | CB  | GLU | A | 533 | 26.502 | 50.013 | 72.130 | 1.00 | 15.68 |
| ATOM | 4241 | CG  | GLU | A | 533 | 25.676 | 49.346 | 71.022 | 1.00 | 16.38 |
| ATOM | 4242 | CD  | GLU | A | 533 | 24.472 | 48.583 | 71.547 | 1.00 | 31.64 |
| ATOM | 4243 | OE1 | GLU | A | 533 | 24.351 | 48.232 | 72.709 | 1.00 | 26.24 |
| ATOM | 4244 | OE2 | GLU | A | 533 | 23.567 | 48.306 | 70.632 | 1.00 | 22.18 |
| ATOM | 4245 | N   | ILE | A | 534 | 27.623 | 52.323 | 73.715 | 1.00 | 16.64 |
| ATOM | 4246 | CA  | ILE | A | 534 | 28.399 | 52.848 | 74.844 | 1.00 | 15.19 |
| ATOM | 4247 | C   | ILE | A | 534 | 27.683 | 53.998 |        |      |       |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 4263 | NH2 | ARG | A | 535 | 25.687 | 62.706 | 75.647 | 1.00 | 22.19 |
| ATOM | 4264 | N   | PHE | A | 536 | 24.536 | 54.737 | 75.575 | 1.00 | 13.92 |
| ATOM | 4265 | CA  | PHE | A | 536 | 23.389 | 54.204 | 76.215 | 1.00 | 12.79 |
| ATOM | 4266 | C   | PHE | A | 536 | 23.740 | 53.693 | 77.615 | 1.00 | 14.46 |
| ATOM | 4267 | O   | PHE | A | 536 | 23.149 | 54.108 | 78.611 | 1.00 | 16.15 |
| ATOM | 4268 | CB  | PHE | A | 536 | 22.900 | 53.039 | 75.342 | 1.00 | 15.26 |
| ATOM | 4269 | CG  | PHE | A | 536 | 21.850 | 52.203 | 76.023 | 1.00 | 16.37 |
| ATOM | 4270 | CD1 | PHE | A | 536 | 20.709 | 52.802 | 76.552 | 1.00 | 16.83 |
| ATOM | 4271 | CD2 | PHE | A | 536 | 21.994 | 50.824 | 76.169 | 1.00 | 19.63 |
| ATOM | 4272 | CE1 | PHE | A | 536 | 19.722 | 52.046 | 77.174 | 1.00 | 16.86 |
| ATOM | 4273 | CE2 | PHE | A | 536 | 21.021 | 50.049 | 76.803 | 1.00 | 20.21 |
| ATOM | 4274 | CZ  | PHE | A | 536 | 19.882 | 50.670 | 77.316 | 1.00 | 17.52 |
| ATOM | 4275 | N   | ARG | A | 537 | 24.690 | 52.747 | 77.674 | 1.00 | 11.77 |
| ATOM | 4276 | CA  | ARG | A | 537 | 25.105 | 52.121 | 78.937 | 1.00 | 11.76 |
| ATOM | 4277 | C   | ARG | A | 537 | 25.696 | 53.100 | 79.956 | 1.00 | 18.24 |
| ATOM | 4278 | O   | ARG | A | 537 | 25.473 | 52.999 | 81.174 | 1.00 | 17.20 |
| ATOM | 4279 | CB  | ARG | A | 537 | 26.019 | 50.937 | 78.709 | 1.00 | 13.64 |
| ATOM | 4280 | CG  | ARG | A | 537 | 25.267 | 49.722 | 78.148 | 1.00 | 13.64 |
| ATOM | 4281 | CD  | ARG | A | 537 | 26.131 | 48.455 | 77.966 | 1.00 | 15.77 |
| ATOM | 4282 | NE  | ARG | A | 537 | 25.256 | 47.437 | 77.410 | 1.00 | 15.36 |
| ATOM | 4283 | CZ  | ARG | A | 537 | 24.877 | 47.385 | 76.148 | 1.00 | 21.63 |
| ATOM | 4284 | NH1 | ARG | A | 537 | 25.365 | 48.200 | 75.215 | 1.00 | 14.82 |
| ATOM | 4285 | NH2 | ARG | A | 537 | 23.988 | 46.465 | 75.821 | 1.00 | 20.40 |
| ATOM | 4286 | N   | TRP | A | 538 | 26.472 | 54.053 | 79.436 | 1.00 | 13.41 |
| ATOM | 4287 | CA  | TRP | A | 538 | 27.065 | 55.079 | 80.266 | 1.00 | 13.47 |
| ATOM | 4288 | C   | TRP | A | 538 | 25.957 | 55.943 | 80.903 | 1.00 | 17.87 |
| ATOM | 4289 | O   | TRP | A | 538 | 25.954 | 56.171 | 82.099 | 1.00 | 16.80 |
| ATOM | 4290 | CB  | TRP | A | 538 | 28.037 | 55.924 | 79.407 | 1.00 | 11.54 |
| ATOM | 4291 | CG  | TRP | A | 538 | 28.492 | 57.235 | 80.033 | 1.00 | 12.21 |
| ATOM | 4292 | CD1 | TRP | A | 538 | 28.350 | 58.451 | 79.472 | 1.00 | 15.63 |
| ATOM | 4293 | CD2 | TRP | A | 538 | 29.203 | 57.461 | 81.276 | 1.00 | 11.84 |
| ATOM | 4294 | NE1 | TRP | A | 538 | 28.889 | 59.415 | 80.286 | 1.00 | 15.48 |
| ATOM | 4295 | CE2 | TRP | A | 538 | 29.428 | 58.838 | 81.379 | 1.00 | 15.91 |
| ATOM | 4296 | CE3 | TRP | A | 538 | 29.634 | 56.621 | 82.304 | 1.00 | 13.93 |
| ATOM | 4297 | CZ2 | TRP | A | 538 | 30.064 | 59.418 | 82.466 | 1.00 | 16.48 |
| ATOM | 4298 | CZ3 | TRP | A | 538 | 30.278 | 57.180 | 83.382 | 1.00 | 15.59 |
| ATOM | 4299 | CH2 | TRP | A | 538 | 30.489 | 58.571 | 83.461 | 1.00 | 16.98 |
| ATOM | 4300 | N   | LEU | A | 539 | 24.995 | 56.427 | 80.100 | 1.00 | 13.56 |
| ATOM | 4301 | CA  | LEU | A | 539 | 23.950 | 57.251 | 80.649 | 1.00 | 13.46 |
| ATOM | 4302 | C   | LEU | A | 539 | 23.109 | 56.517 | 81.690 | 1.00 | 16.76 |
| ATOM | 4303 | O   | LEU | A | 539 | 22.704 | 57.102 | 82.675 | 1.00 | 17.06 |
| ATOM | 4304 | CB  | LEU | A | 539 | 23.074 | 57.929 | 79.554 | 1.00 | 15.88 |
| ATOM | 4305 | CG  | LEU | A | 539 | 23.865 | 58.813 | 78.563 | 1.00 | 16.07 |
| ATOM | 4306 | CD1 | LEU | A | 539 | 22.966 | 59.449 | 77.529 | 1.00 | 16.70 |
| ATOM | 4307 | CD2 | LEU | A | 539 | 24.614 | 59.889 | 79.304 | 1.00 | 14.42 |
| ATOM | 4308 | N   | ARG | A | 540 | 22.856 | 55.223 | 81.481 | 1.00 | 16.81 |
| ATOM | 4309 | CA  | ARG | A | 540 | 22.096 | 54.425 | 82.436 | 1.00 | 16.05 |
| ATOM | 4310 | C   | ARG | A | 540 | 22.821 | 54.404 | 83.764 | 1.00 | 18.54 |
| ATOM | 4311 | O   | ARG | A | 540 | 22.263 | 54.664 | 84.821 | 1.00 | 20.40 |
| ATOM | 4312 | CB  | ARG | A | 540 | 21.887 | 52.973 | 81.974 | 1.00 | 15.71 |
| ATOM | 4313 | CG  | ARG | A | 540 | 21.026 | 52.845 | 80.716 | 1.00 | 19.20 |
| ATOM | 4314 | CD  | ARG | A | 540 | 20.461 | 51.430 | 80.612 | 1.00 | 21.64 |
| ATOM | 4315 | NE  | ARG | A | 540 | 19.576 | 51.166 | 81.748 | 1.00 | 21.09 |
| ATOM | 4316 | CZ  | ARG | A | 540 | 18.903 | 50.051 | 81.977 | 1.00 | 30.30 |
| ATOM | 4317 | NH1 | ARG | A | 540 | 19.003 | 49.003 | 81.176 | 1.00 | 22.34 |
| ATOM | 4318 | NH2 | ARG | A | 540 | 18.101 | 49.987 | 83.047 | 1.00 | 32.88 |
| ATOM | 4319 | N   | LEU | A | 541 | 24.093 | 54.091 | 83.685 | 1.00 | 12.62 |
| ATOM | 4320 | CA  | LEU | A | 541 | 24.942 | 54.027 | 84.860 | 1.00 | 13.44 |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 4321 | C   | LEU | A | 541 | 24.921 | 55.334 | 85.630 | 1.00 | 19.38 |
| ATOM | 4322 | O   | LEU | A | 541 | 24.891 | 55.375 | 86.850 | 1.00 | 18.05 |
| ATOM | 4323 | CB  | LEU | A | 541 | 26.389 | 53.723 | 84.435 | 1.00 | 14.55 |
| ATOM | 4324 | CG  | LEU | A | 541 | 27.377 | 53.612 | 85.612 | 1.00 | 17.61 |
| ATOM | 4325 | CD1 | LEU | A | 541 | 26.967 | 52.499 | 86.584 | 1.00 | 14.91 |
| ATOM | 4326 | CD2 | LEU | A | 541 | 28.783 | 53.322 | 85.082 | 1.00 | 13.20 |
| ATOM | 4327 | N   | CYS | A | 542 | 24.948 | 56.425 | 84.883 | 1.00 | 18.18 |
| ATOM | 4328 | CA  | CYS | A | 542 | 24.927 | 57.747 | 85.455 | 1.00 | 16.56 |
| ATOM | 4329 | C   | CYS | A | 542 | 23.589 | 58.013 | 86.138 | 1.00 | 17.68 |
| ATOM | 4330 | O   | CYS | A | 542 | 23.550 | 58.514 | 87.247 | 1.00 | 17.12 |
| ATOM | 4331 | CB  | CYS | A | 542 | 25.159 | 58.811 | 84.353 | 1.00 | 16.15 |
| ATOM | 4332 | SG  | CYS | A | 542 | 26.884 | 58.903 | 83.797 | 1.00 | 18.89 |
| ATOM | 4333 | N   | ILE | A | 543 | 22.485 | 57.696 | 85.448 | 1.00 | 15.90 |
| ATOM | 4334 | CA  | ILE | A | 543 | 21.158 | 57.935 | 85.991 | 1.00 | 15.89 |
| ATOM | 4335 | C   | ILE | A | 543 | 20.912 | 57.085 | 87.207 | 1.00 | 19.52 |
| ATOM | 4336 | O   | ILE | A | 543 | 20.450 | 57.530 | 88.248 | 1.00 | 14.90 |
| ATOM | 4337 | CB  | ILE | A | 543 | 20.089 | 57.759 | 84.922 | 1.00 | 16.53 |
| ATOM | 4338 | CG1 | ILE | A | 543 | 20.267 | 58.837 | 83.862 | 1.00 | 16.25 |
| ATOM | 4339 | CG2 | ILE | A | 543 | 18.719 | 57.890 | 85.524 | 1.00 | 13.95 |
| ATOM | 4340 | CD1 | ILE | A | 543 | 20.224 | 60.275 | 84.423 | 1.00 | 23.20 |
| ATOM | 4341 | N   | GLN | A | 544 | 21.265 | 55.846 | 87.062 | 1.00 | 16.81 |
| ATOM | 4342 | CA  | GLN | A | 544 | 21.083 | 54.915 | 88.140 | 1.00 | 16.91 |
| ATOM | 4343 | C   | GLN | A | 544 | 21.919 | 55.264 | 89.338 | 1.00 | 21.44 |
| ATOM | 4344 | O   | GLN | A | 544 | 21.560 | 54.872 | 90.464 | 1.00 | 17.71 |
| ATOM | 4345 | CB  | GLN | A | 544 | 21.329 | 53.469 | 87.676 | 1.00 | 17.14 |
| ATOM | 4346 | CG  | GLN | A | 544 | 20.245 | 53.073 | 86.660 | 1.00 | 16.46 |
| ATOM | 4347 | CD  | GLN | A | 544 | 20.353 | 51.658 | 86.156 | 1.00 | 18.46 |
| ATOM | 4348 | OE1 | GLN | A | 544 | 19.958 | 51.363 | 85.017 | 1.00 | 29.64 |
| ATOM | 4349 | NE2 | GLN | A | 544 | 20.821 | 50.768 | 87.006 | 1.00 | 14.23 |
| ATOM | 4350 | N   | SER | A | 545 | 23.022 | 56.011 | 89.083 | 1.00 | 16.96 |
| ATOM | 4351 | CA  | SER | A | 545 | 23.920 | 56.419 | 90.172 | 1.00 | 16.35 |
| ATOM | 4352 | C   | SER | A | 545 | 23.576 | 57.773 | 90.757 | 1.00 | 21.69 |
| ATOM | 4353 | O   | SER | A | 545 | 24.314 | 58.320 | 91.571 | 1.00 | 20.97 |
| ATOM | 4354 | CB  | SER | A | 545 | 25.389 | 56.331 | 89.822 | 1.00 | 14.78 |
| ATOM | 4355 | OG  | SER | A | 545 | 25.645 | 54.989 | 89.461 | 1.00 | 16.47 |
| ATOM | 4356 | N   | LYS | A | 546 | 22.445 | 58.295 | 90.299 | 1.00 | 19.83 |
| ATOM | 4357 | CA  | LYS | A | 546 | 21.919 | 59.553 | 90.748 | 1.00 | 18.17 |
| ATOM | 4358 | C   | LYS | A | 546 | 22.682 | 60.775 | 90.346 | 1.00 | 20.74 |
| ATOM | 4359 | O   | LYS | A | 546 | 22.744 | 61.705 | 91.136 | 1.00 | 20.74 |
| ATOM | 4360 | CB  | LYS | A | 546 | 21.757 | 59.578 | 92.245 | 1.00 | 17.98 |
| ATOM | 4361 | CG  | LYS | A | 546 | 21.192 | 58.279 | 92.761 | 1.00 | 19.40 |
| ATOM | 4362 | CD  | LYS | A | 546 | 19.811 | 57.972 | 92.190 | 1.00 | 24.16 |
| ATOM | 4363 | CE  | LYS | A | 546 | 19.182 | 56.724 | 92.840 | 1.00 | 30.41 |
| ATOM | 4364 | NZ  | LYS | A | 546 | 17.911 | 56.281 | 92.237 | 1.00 | 21.29 |
| ATOM | 4365 | N   | TRP | A | 547 | 23.227 | 60.817 | 89.147 | 1.00 | 16.41 |
| ATOM | 4366 | CA  | TRP | A | 547 | 23.944 | 61.999 | 88.742 | 1.00 | 15.28 |
| ATOM | 4367 | C   | TRP | A | 547 | 23.027 | 62.921 | 88.034 | 1.00 | 20.17 |
| ATOM | 4368 | O   | TRP | A | 547 | 22.649 | 62.672 | 86.908 | 1.00 | 20.03 |
| ATOM | 4369 | CB  | TRP | A | 547 | 25.133 | 61.647 | 87.854 | 1.00 | 15.66 |
| ATOM | 4370 | CG  | TRP | A | 547 | 26.127 | 62.755 | 87.670 | 1.00 | 15.61 |
| ATOM | 4371 | CD1 | TRP | A | 547 | 26.146 | 63.957 | 88.330 | 1.00 | 18.93 |
| ATOM | 4372 | CD2 | TRP | A | 547 | 27.249 | 62.756 | 86.796 | 1.00 | 14.82 |
| ATOM | 4373 | NE1 | TRP | A | 547 | 27.232 | 64.678 | 87.930 | 1.00 | 18.02 |
| ATOM | 4374 | CE2 | TRP | A | 547 | 27.923 | 63.965 | 86.989 | 1.00 | 18.89 |
| ATOM | 4375 | CE3 | TRP | A | 547 | 27.763 | 61.827 | 85.888 | 1.00 | 18.21 |
| ATOM | 4376 | CZ2 | TRP | A | 547 | 29.068 | 64.290 | 86.254 | 1.00 | 19.21 |
| ATOM | 4377 | CZ3 | TRP | A | 547 | 28.903 | 62.124 | 85.188 | 1.00 | 20.09 |
| ATOM | 4378 | CH2 | TRP | A | 547 | 29.553 | 63.343 | 85.365 | 1.00 | 20.78 |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 4379 | N   | GLU | A | 548 | 22.658 | 64.011 | 88.682 | 1.00 | 16.10 |
| ATOM | 4380 | CA  | GLU | A | 548 | 21.761 | 64.914 | 88.029 | 1.00 | 17.50 |
| ATOM | 4381 | C   | GLU | A | 548 | 22.257 | 65.492 | 86.730 | 1.00 | 19.53 |
| ATOM | 4382 | O   | GLU | A | 548 | 21.456 | 65.804 | 85.870 | 1.00 | 19.12 |
| ATOM | 4383 | CB  | GLU | A | 548 | 21.247 | 66.016 | 88.969 | 1.00 | 19.98 |
| ATOM | 4384 | CG  | GLU | A | 548 | 20.555 | 65.419 | 90.229 | 1.00 | 24.06 |
| ATOM | 4385 | CD  | GLU | A | 548 | 20.077 | 66.445 | 91.243 | 1.00 | 33.90 |
| ATOM | 4386 | OE1 | GLU | A | 548 | 19.441 | 67.440 | 90.965 | 1.00 | 43.66 |
| ATOM | 4387 | OE2 | GLU | A | 548 | 20.393 | 66.129 | 92.465 | 1.00 | 43.45 |
| ATOM | 4388 | N   | ASP | A | 549 | 23.555 | 65.667 | 86.569 | 1.00 | 16.60 |
| ATOM | 4389 | CA  | ASP | A | 549 | 24.054 | 66.258 | 85.351 | 1.00 | 14.55 |
| ATOM | 4390 | C   | ASP | A | 549 | 23.736 | 65.449 | 84.132 | 1.00 | 18.68 |
| ATOM | 4391 | O   | ASP | A | 549 | 23.663 | 65.937 | 82.985 | 1.00 | 18.55 |
| ATOM | 4392 | CB  | ASP | A | 549 | 25.554 | 66.515 | 85.439 | 1.00 | 15.80 |
| ATOM | 4393 | CG  | ASP | A | 549 | 25.809 | 67.504 | 86.537 | 1.00 | 31.75 |
| ATOM | 4394 | OD1 | ASP | A | 549 | 25.557 | 68.672 | 86.421 | 1.00 | 37.38 |
| ATOM | 4395 | OD2 | ASP | A | 549 | 26.188 | 66.966 | 87.658 | 1.00 | 56.37 |
| ATOM | 4396 | N   | ALA | A | 550 | 23.531 | 64.199 | 84.392 | 1.00 | 15.83 |
| ATOM | 4397 | CA  | ALA | A | 550 | 23.243 | 63.296 | 83.304 | 1.00 | 16.81 |
| ATOM | 4398 | C   | ALA | A | 550 | 21.793 | 63.312 | 82.827 | 1.00 | 22.33 |
| ATOM | 4399 | O   | ALA | A | 550 | 21.496 | 62.708 | 81.787 | 1.00 | 22.90 |
| ATOM | 4400 | CB  | ALA | A | 550 | 23.681 | 61.866 | 83.678 | 1.00 | 15.17 |
| ATOM | 4401 | N   | ILE | A | 551 | 20.885 | 63.965 | 83.563 | 1.00 | 17.67 |
| ATOM | 4402 | CA  | ILE | A | 551 | 19.468 | 63.990 | 83.178 | 1.00 | 17.00 |
| ATOM | 4403 | C   | ILE | A | 551 | 19.205 | 64.533 | 81.787 | 1.00 | 19.27 |
| ATOM | 4404 | O   | ILE | A | 551 | 18.489 | 63.951 | 80.967 | 1.00 | 19.75 |
| ATOM | 4405 | CB  | ILE | A | 551 | 18.660 | 64.767 | 84.195 | 1.00 | 20.59 |
| ATOM | 4406 | CG1 | ILE | A | 551 | 18.688 | 64.024 | 85.537 | 1.00 | 20.00 |
| ATOM | 4407 | CG2 | ILE | A | 551 | 17.234 | 65.035 | 83.688 | 1.00 | 17.64 |
| ATOM | 4408 | CD1 | ILE | A | 551 | 18.004 | 64.753 | 86.709 | 1.00 | 22.00 |
| ATOM | 4409 | N   | PRO | A | 552 | 19.786 | 65.669 | 81.492 | 1.00 | 18.31 |
| ATOM | 4410 | CA  | PRO | A | 552 | 19.587 | 66.261 | 80.192 | 1.00 | 18.26 |
| ATOM | 4411 | C   | PRO | A | 552 | 20.131 | 65.378 | 79.089 | 1.00 | 19.47 |
| ATOM | 4412 | O   | PRO | A | 552 | 19.542 | 65.280 | 78.001 | 1.00 | 19.84 |
| ATOM | 4413 | CB  | PRO | A | 552 | 20.313 | 67.600 | 80.184 | 1.00 | 20.28 |
| ATOM | 4414 | CG  | PRO | A | 552 | 21.074 | 67.684 | 81.493 | 1.00 | 25.73 |
| ATOM | 4415 | CD  | PRO | A | 552 | 20.636 | 66.508 | 82.349 | 1.00 | 20.00 |
| ATOM | 4416 | N   | LEU | A | 553 | 21.255 | 64.732 | 79.344 | 1.00 | 15.41 |
| ATOM | 4417 | CA  | LEU | A | 553 | 21.827 | 63.866 | 78.302 | 1.00 | 16.23 |
| ATOM | 4418 | C   | LEU | A | 553 | 20.953 | 62.634 | 78.024 | 1.00 | 22.52 |
| ATOM | 4419 | O   | LEU | A | 553 | 20.787 | 62.169 | 76.889 | 1.00 | 21.48 |
| ATOM | 4420 | CB  | LEU | A | 553 | 23.235 | 63.408 | 78.700 | 1.00 | 16.94 |
| ATOM | 4421 | CG  | LEU | A | 553 | 24.171 | 64.557 | 79.088 | 1.00 | 22.66 |
| ATOM | 4422 | CD1 | LEU | A | 553 | 25.563 | 63.989 | 79.402 | 1.00 | 20.12 |
| ATOM | 4423 | CD2 | LEU | A | 553 | 24.288 | 65.558 | 77.934 | 1.00 | 24.27 |
| ATOM | 4424 | N   | ALA | A | 554 | 20.407 | 62.088 | 79.094 | 1.00 | 19.11 |
| ATOM | 4425 | CA  | ALA | A | 554 | 19.586 | 60.907 | 78.982 | 1.00 | 15.78 |
| ATOM | 4426 | C   | ALA | A | 554 | 18.288 | 61.247 | 78.315 | 1.00 | 18.70 |
| ATOM | 4427 | O   | ALA | A | 554 | 17.822 | 60.504 | 77.457 | 1.00 | 18.11 |
| ATOM | 4428 | CB  | ALA | A | 554 | 19.372 | 60.252 | 80.325 | 1.00 | 13.78 |
| ATOM | 4429 | N   | LEU | A | 555 | 17.711 | 62.384 | 78.695 | 1.00 | 14.55 |
| ATOM | 4430 | CA  | LEU | A | 555 | 16.450 | 62.765 | 78.083 | 1.00 | 16.26 |
| ATOM | 4431 | C   | LEU | A | 555 | 16.624 | 63.002 | 76.596 | 1.00 | 21.06 |
| ATOM | 4432 | O   | LEU | A | 555 | 15.757 | 62.691 | 75.774 | 1.00 | 19.79 |
| ATOM | 4433 | CB  | LEU | A | 555 | 15.895 | 64.065 | 78.654 | 1.00 | 16.61 |
| ATOM | 4434 | CG  | LEU | A | 555 | 15.266 | 63.935 | 80.034 | 1.00 | 25.68 |
| ATOM | 4435 | CD1 | LEU | A | 555 | 15.074 | 65.355 | 80.626 | 1.00 | 25.00 |
| ATOM | 4436 | CD2 | LEU | A | 555 | 13.931 | 63.190 | 79.901 | 1.00 | 26.60 |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 4437 | N   | LYS | A | 556 | 17.770 | 63.597 | 76.263 | 1.00 | 19.69 |
| ATOM | 4438 | CA  | LYS | A | 556 | 18.092 | 63.918 | 74.886 | 1.00 | 17.75 |
| ATOM | 4439 | C   | LYS | A | 556 | 18.260 | 62.667 | 74.065 | 1.00 | 20.15 |
| ATOM | 4440 | O   | LYS | A | 556 | 17.727 | 62.531 | 72.962 | 1.00 | 20.20 |
| ATOM | 4441 | CB  | LYS | A | 556 | 19.343 | 64.773 | 74.847 | 1.00 | 21.25 |
| ATOM | 4442 | CG  | LYS | A | 556 | 19.518 | 65.514 | 73.537 | 1.00 | 57.55 |
| ATOM | 4443 | CD  | LYS | A | 556 | 20.912 | 65.351 | 72.936 | 1.00 | 78.14 |
| ATOM | 4444 | CE  | LYS | A | 556 | 21.873 | 66.491 | 73.247 | 1.00 | 85.39 |
| ATOM | 4445 | NZ  | LYS | A | 556 | 22.965 | 66.584 | 72.261 | 1.00 | 90.20 |
| ATOM | 4446 | N   | MET | A | 557 | 19.011 | 61.732 | 74.607 | 1.00 | 16.39 |
| ATOM | 4447 | CA  | MET | A | 557 | 19.241 | 60.514 | 73.863 | 1.00 | 16.19 |
| ATOM | 4448 | C   | MET | A | 557 | 17.948 | 59.731 | 73.605 | 1.00 | 22.82 |
| ATOM | 4449 | O   | MET | A | 557 | 17.714 | 59.142 | 72.523 | 1.00 | 19.87 |
| ATOM | 4450 | CB  | MET | A | 557 | 20.286 | 59.635 | 74.589 | 1.00 | 17.35 |
| ATOM | 4451 | CG  | MET | A | 557 | 20.489 | 58.320 | 73.829 | 1.00 | 20.22 |
| ATOM | 4452 | SD  | MET | A | 557 | 21.933 | 57.357 | 74.325 | 1.00 | 22.67 |
| ATOM | 4453 | CE  | MET | A | 557 | 21.962 | 56.107 | 73.009 | 1.00 | 16.66 |
| ATOM | 4454 | N   | ALA | A | 558 | 17.110 | 59.724 | 74.644 | 1.00 | 18.95 |
| ATOM | 4455 | CA  | ALA | A | 558 | 15.857 | 59.013 | 74.607 | 1.00 | 20.49 |
| ATOM | 4456 | C   | ALA | A | 558 | 14.856 | 59.525 | 73.592 | 1.00 | 27.56 |
| ATOM | 4457 | O   | ALA | A | 558 | 14.019 | 58.768 | 73.100 | 1.00 | 25.54 |
| ATOM | 4458 | CB  | ALA | A | 558 | 15.223 | 58.968 | 75.988 | 1.00 | 19.57 |
| ATOM | 4459 | N   | THR | A | 559 | 14.933 | 60.811 | 73.295 | 1.00 | 22.11 |
| ATOM | 4460 | CA  | THR | A | 559 | 13.967 | 61.381 | 72.407 | 1.00 | 20.16 |
| ATOM | 4461 | C   | THR | A | 559 | 14.539 | 61.680 | 71.057 | 1.00 | 22.76 |
| ATOM | 4462 | O   | THR | A | 559 | 13.797 | 61.814 | 70.094 | 1.00 | 24.26 |
| ATOM | 4463 | CB  | THR | A | 559 | 13.369 | 62.652 | 73.069 | 1.00 | 24.38 |
| ATOM | 4464 | OG1 | THR | A | 559 | 14.413 | 63.571 | 73.345 | 1.00 | 22.44 |
| ATOM | 4465 | CG2 | THR | A | 559 | 12.691 | 62.323 | 74.399 | 1.00 | 20.52 |
| ATOM | 4466 | N   | GLU | A | 560 | 15.844 | 61.818 | 70.974 | 1.00 | 20.87 |
| ATOM | 4467 | CA  | GLU | A | 560 | 16.484 | 62.130 | 69.690 | 1.00 | 22.00 |
| ATOM | 4468 | C   | GLU | A | 560 | 16.577 | 60.919 | 68.736 | 1.00 | 24.16 |
| ATOM | 4469 | O   | GLU | A | 560 | 16.808 | 61.067 | 67.544 | 1.00 | 21.97 |
| ATOM | 4470 | CB  | GLU | A | 560 | 17.886 | 62.698 | 69.862 | 1.00 | 24.33 |
| ATOM | 4471 | CG  | GLU | A | 560 | 17.972 | 64.085 | 70.540 | 1.00 | 45.69 |
| ATOM | 4472 | CD  | GLU | A | 560 | 19.325 | 64.716 | 70.282 | 1.00 | 59.21 |
| ATOM | 4473 | OE1 | GLU | A | 560 | 20.368 | 64.080 | 70.224 | 1.00 | 76.40 |
| ATOM | 4474 | OE2 | GLU | A | 560 | 19.242 | 66.006 | 70.150 | 1.00 | 50.76 |
| ATOM | 4475 | N   | GLN | A | 561 | 16.443 | 59.733 | 69.302 | 1.00 | 18.19 |
| ATOM | 4476 | CA  | GLN | A | 561 | 16.435 | 58.488 | 68.551 | 1.00 | 18.56 |
| ATOM | 4477 | C   | GLN | A | 561 | 15.316 | 57.658 | 69.172 | 1.00 | 24.31 |
| ATOM | 4478 | O   | GLN | A | 561 | 14.881 | 57.985 | 70.297 | 1.00 | 21.89 |
| ATOM | 4479 | CB  | GLN | A | 561 | 17.796 |        |        |      |       |



6042210-02699

|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 4495 | NE  | ARG | A | 563 | 19.313 | 49.407 | 68.387 | 1.00 | 18.90 |
| ATOM | 4496 | CZ  | ARG | A | 563 | 20.573 | 49.140 | 68.134 | 1.00 | 24.90 |
| ATOM | 4497 | NH1 | ARG | A | 563 | 21.436 | 50.117 | 67.850 | 1.00 | 21.86 |
| ATOM | 4498 | NH2 | ARG | A | 563 | 20.970 | 47.875 | 68.121 | 1.00 | 25.10 |
| ATOM | 4499 | N   | MET | A | 564 | 13.983 | 51.212 | 70.448 | 1.00 | 18.13 |
| ATOM | 4500 | CA  | MET | A | 564 | 13.425 | 50.773 | 71.729 | 1.00 | 17.97 |
| ATOM | 4501 | C   | MET | A | 564 | 14.436 | 50.274 | 72.756 | 1.00 | 21.65 |
| ATOM | 4502 | O   | MET | A | 564 | 14.291 | 50.503 | 73.958 | 1.00 | 19.02 |
| ATOM | 4503 | CB  | MET | A | 564 | 12.231 | 49.809 | 71.540 | 1.00 | 18.77 |
| ATOM | 4504 | CG  | MET | A | 564 | 11.120 | 50.498 | 70.779 | 1.00 | 22.52 |
| ATOM | 4505 | SD  | MET | A | 564 | 9.651  | 49.485 | 70.814 | 1.00 | 30.74 |
| ATOM | 4506 | CE  | MET | A | 564 | 10.140 | 48.213 | 69.638 | 1.00 | 26.15 |
| ATOM | 4507 | N   | LYS | A | 565 | 15.446 | 49.560 | 72.248 | 1.00 | 18.83 |
| ATOM | 4508 | CA  | LYS | A | 565 | 16.540 | 49.011 | 73.032 | 1.00 | 19.08 |
| ATOM | 4509 | C   | LYS | A | 565 | 17.141 | 50.110 | 73.924 | 1.00 | 18.89 |
| ATOM | 4510 | O   | LYS | A | 565 | 17.592 | 49.852 | 75.027 | 1.00 | 16.93 |
| ATOM | 4511 | CB  | LYS | A | 565 | 17.595 | 48.485 | 72.063 | 1.00 | 15.54 |
| ATOM | 4512 | CG  | LYS | A | 565 | 18.769 | 47.873 | 72.740 | 1.00 | 20.37 |
| ATOM | 4513 | CD  | LYS | A | 565 | 19.871 | 47.486 | 71.768 | 1.00 | 19.32 |
| ATOM | 4514 | CE  | LYS | A | 565 | 20.892 | 46.604 | 72.452 | 1.00 | 27.76 |
| ATOM | 4515 | NZ  | LYS | A | 565 | 22.112 | 46.360 | 71.670 | 1.00 | 21.11 |
| ATOM | 4516 | N   | PHE | A | 566 | 17.142 | 51.345 | 73.423 | 1.00 | 14.76 |
| ATOM | 4517 | CA  | PHE | A | 566 | 17.708 | 52.462 | 74.159 | 1.00 | 13.39 |
| ATOM | 4518 | C   | PHE | A | 566 | 16.651 | 53.323 | 74.834 | 1.00 | 17.12 |
| ATOM | 4519 | O   | PHE | A | 566 | 16.733 | 53.674 | 76.007 | 1.00 | 14.88 |
| ATOM | 4520 | CB  | PHE | A | 566 | 18.580 | 53.378 | 73.266 | 1.00 | 12.33 |
| ATOM | 4521 | CG  | PHE | A | 566 | 19.692 | 52.683 | 72.484 | 1.00 | 14.16 |
| ATOM | 4522 | CD1 | PHE | A | 566 | 20.411 | 51.604 | 73.016 | 1.00 | 15.94 |
| ATOM | 4523 | CD2 | PHE | A | 566 | 20.015 | 53.131 | 71.193 | 1.00 | 16.01 |
| ATOM | 4524 | CE1 | PHE | A | 566 | 21.421 | 50.974 | 72.277 | 1.00 | 15.47 |
| ATOM | 4525 | CE2 | PHE | A | 566 | 21.018 | 52.522 | 70.431 | 1.00 | 14.85 |
| ATOM | 4526 | CZ  | PHE | A | 566 | 21.713 | 51.444 | 70.991 | 1.00 | 15.39 |
| ATOM | 4527 | N   | THR | A | 567 | 15.683 | 53.708 | 74.040 | 1.00 | 16.88 |
| ATOM | 4528 | CA  | THR | A | 567 | 14.608 | 54.584 | 74.493 | 1.00 | 15.59 |
| ATOM | 4529 | C   | THR | A | 567 | 13.824 | 54.079 | 75.697 | 1.00 | 17.49 |
| ATOM | 4530 | O   | THR | A | 567 | 13.596 | 54.845 | 76.653 | 1.00 | 17.50 |
| ATOM | 4531 | CB  | THR | A | 567 | 13.683 | 54.960 | 73.329 | 1.00 | 18.44 |
| ATOM | 4532 | OG1 | THR | A | 567 | 14.397 | 55.788 | 72.420 | 1.00 | 17.49 |
| ATOM | 4533 | CG2 | THR | A | 567 | 12.423 | 55.652 | 73.866 | 1.00 | 20.99 |
| ATOM | 4534 | N   | ARG | A | 568 | 13.411 | 52.800 | 75.655 | 1.00 | 14.94 |
| ATOM | 4535 | CA  | ARG | A | 568 | 12.639 | 52.235 | 76.761 | 1.00 | 15.43 |
| ATOM | 4536 | C   | ARG | A | 568 | 13.335 | 52.286 | 78.121 | 1.00 | 18.16 |
| ATOM | 4537 | O   | ARG | A | 568 | 12.789 | 52.796 | 79.084 | 1.00 | 16.87 |
| ATOM | 4538 | CB  | ARG | A | 568 | 12.071 | 50.875 | 76.423 | 1.00 | 13.94 |
| ATOM | 4539 | CG  | ARG | A | 568 | 11.026 | 51.000 | 75.302 | 1.00 | 11.32 |
| ATOM | 4540 | CD  | ARG | A | 568 | 10.386 | 49.656 | 74.991 | 1.00 | 14.79 |
| ATOM | 4541 | NE  | ARG | A | 568 | 9.659  | 49.172 | 76.147 | 1.00 | 18.40 |
| ATOM | 4542 | CZ  | ARG | A | 568 | 9.166  | 47.960 | 76.287 | 1.00 | 25.32 |
| ATOM | 4543 | NH1 | ARG | A | 568 | 9.322  | 47.012 | 75.354 | 1.00 | 16.84 |
| ATOM | 4544 | NH2 | ARG | A | 568 | 8.496  | 47.696 | 77.410 | 1.00 | 16.63 |
| ATOM | 4545 | N   | PRO | A | 569 | 14.548 | 51.776 | 78.168 | 1.00 | 14.13 |
| ATOM | 4546 | CA  | PRO | A | 569 | 15.334 | 51.744 | 79.400 | 1.00 | 16.57 |
| ATOM | 4547 | C   | PRO | A | 569 | 15.749 | 53.092 | 79.904 | 1.00 | 18.71 |
| ATOM | 4548 | O   | PRO | A | 569 | 15.827 | 53.337 | 81.125 | 1.00 | 17.63 |
| ATOM | 4549 | CB  | PRO | A | 569 | 16.576 | 50.883 | 79.101 | 1.00 | 19.20 |
| ATOM | 4550 | CG  | PRO | A | 569 | 16.246 | 50.089 | 77.834 | 1.00 | 19.00 |
| ATOM | 4551 | CD  | PRO | A | 569 | 15.150 | 50.887 | 77.122 | 1.00 | 15.84 |
| ATOM | 4552 | N   | LEU | A | 570 | 16.001 | 53.996 | 78.973 | 1.00 | 16.41 |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 4553 | CA  | LEU | A | 570 | 16.379 | 55.355 | 79.382 | 1.00 | 17.76 |
| ATOM | 4554 | C   | LEU | A | 570 | 15.192 | 56.062 | 80.084 | 1.00 | 22.35 |
| ATOM | 4555 | O   | LEU | A | 570 | 15.339 | 56.681 | 81.150 | 1.00 | 20.52 |
| ATOM | 4556 | CB  | LEU | A | 570 | 16.876 | 56.202 | 78.185 | 1.00 | 17.74 |
| ATOM | 4557 | CG  | LEU | A | 570 | 18.296 | 55.843 | 77.759 | 1.00 | 20.79 |
| ATOM | 4558 | CD1 | LEU | A | 570 | 18.664 | 56.566 | 76.470 | 1.00 | 18.50 |
| ATOM | 4559 | CD2 | LEU | A | 570 | 19.279 | 56.172 | 78.884 | 1.00 | 20.34 |
| ATOM | 4560 | N   | PHE | A | 571 | 14.005 | 55.963 | 79.462 | 1.00 | 17.16 |
| ATOM | 4561 | CA  | PHE | A | 571 | 12.826 | 56.555 | 80.047 | 1.00 | 17.72 |
| ATOM | 4562 | C   | PHE | A | 571 | 12.554 | 55.878 | 81.375 | 1.00 | 19.55 |
| ATOM | 4563 | O   | PHE | A | 571 | 12.169 | 56.500 | 82.372 | 1.00 | 24.27 |
| ATOM | 4564 | CB  | PHE | A | 571 | 11.594 | 56.425 | 79.152 | 1.00 | 18.46 |
| ATOM | 4565 | CG  | PHE | A | 571 | 11.415 | 57.641 | 78.282 | 1.00 | 18.32 |
| ATOM | 4566 | CD1 | PHE | A | 571 | 11.028 | 58.863 | 78.832 | 1.00 | 16.11 |
| ATOM | 4567 | CD2 | PHE | A | 571 | 11.600 | 57.569 | 76.902 | 1.00 | 18.39 |
| ATOM | 4568 | CE1 | PHE | A | 571 | 10.842 | 59.978 | 78.024 | 1.00 | 17.51 |
| ATOM | 4569 | CE2 | PHE | A | 571 | 11.422 | 58.679 | 76.075 | 1.00 | 20.05 |
| ATOM | 4570 | CZ  | PHE | A | 571 | 11.027 | 59.888 | 76.644 | 1.00 | 19.54 |
| ATOM | 4571 | N   | LYS | A | 572 | 12.776 | 54.599 | 81.388 | 1.00 | 13.24 |
| ATOM | 4572 | CA  | LYS | A | 572 | 12.546 | 53.877 | 82.604 | 1.00 | 17.24 |
| ATOM | 4573 | C   | LYS | A | 572 | 13.501 | 54.286 | 83.726 | 1.00 | 22.30 |
| ATOM | 4574 | O   | LYS | A | 572 | 13.093 | 54.481 | 84.887 | 1.00 | 21.20 |
| ATOM | 4575 | CB  | LYS | A | 572 | 12.453 | 52.388 | 82.395 | 1.00 | 19.92 |
| ATOM | 4576 | CG  | LYS | A | 572 | 11.041 | 51.827 | 82.560 | 1.00 | 39.47 |
| ATOM | 4577 | CD  | LYS | A | 572 | 10.969 | 50.322 | 82.245 | 1.00 | 59.94 |
| ATOM | 4578 | CE  | LYS | A | 572 | 10.997 | 49.992 | 80.743 | 1.00 | 81.81 |
| ATOM | 4579 | NZ  | LYS | A | 572 | 11.621 | 48.696 | 80.395 | 1.00 | 84.56 |
| ATOM | 4580 | N   | ASP | A | 573 | 14.765 | 54.436 | 83.393 | 1.00 | 16.20 |
| ATOM | 4581 | CA  | ASP | A | 573 | 15.705 | 54.847 | 84.435 | 1.00 | 15.22 |
| ATOM | 4582 | C   | ASP | A | 573 | 15.383 | 56.235 | 84.891 | 1.00 | 19.06 |
| ATOM | 4583 | O   | ASP | A | 573 | 15.417 | 56.504 | 86.077 | 1.00 | 18.49 |
| ATOM | 4584 | CB  | ASP | A | 573 | 17.178 | 54.824 | 83.992 | 1.00 | 15.52 |
| ATOM | 4585 | CG  | ASP | A | 573 | 17.694 | 53.409 | 83.853 | 1.00 | 24.76 |
| ATOM | 4586 | OD1 | ASP | A | 573 | 17.057 | 52.435 | 84.197 | 1.00 | 25.70 |
| ATOM | 4587 | OD2 | ASP | A | 573 | 18.888 | 53.321 | 83.312 | 1.00 | 28.57 |
| ATOM | 4588 | N   | LEU | A | 574 | 15.092 | 57.114 | 83.921 | 1.00 | 15.30 |
| ATOM | 4589 | CA  | LEU | A | 574 | 14.779 | 58.489 | 84.243 | 1.00 | 17.34 |
| ATOM | 4590 | C   | LEU | A | 574 | 13.530 | 58.595 | 85.127 | 1.00 | 26.84 |
| ATOM | 4591 | O   | LEU | A | 574 | 13.410 | 59.473 | 86.004 | 1.00 | 25.00 |
| ATOM | 4592 | CB  | LEU | A | 574 | 14.608 | 59.351 | 82.977 | 1.00 | 17.58 |
| ATOM | 4593 | CG  | LEU | A | 574 | 15.900 | 59.592 | 82.190 | 1.00 | 22.57 |
| ATOM | 4594 | CD1 | LEU | A | 574 | 15.486 | 60.046 | 80.797 | 1.00 | 21.18 |
| ATOM | 4595 | CD2 | LEU | A | 574 |        |        |        |      |       |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 4611 | CG  | PHE | A | 577 | 17.388 | 60.135 | 89.029 | 1.00 | 20.29 |
| ATOM | 4612 | CD1 | PHE | A | 577 | 17.608 | 60.272 | 90.405 | 1.00 | 21.38 |
| ATOM | 4613 | CD2 | PHE | A | 577 | 18.181 | 60.895 | 88.160 | 1.00 | 22.30 |
| ATOM | 4614 | CE1 | PHE | A | 577 | 18.591 | 61.145 | 90.888 | 1.00 | 22.36 |
| ATOM | 4615 | CE2 | PHE | A | 577 | 19.169 | 61.769 | 88.622 | 1.00 | 21.90 |
| ATOM | 4616 | CZ  | PHE | A | 577 | 19.364 | 61.899 | 89.998 | 1.00 | 19.38 |
| ATOM | 4617 | N   | ASP | A | 578 | 14.288 | 60.104 | 91.245 | 1.00 | 22.86 |
| ATOM | 4618 | CA  | ASP | A | 578 | 13.434 | 61.134 | 91.791 | 1.00 | 25.52 |
| ATOM | 4619 | C   | ASP | A | 578 | 13.561 | 62.456 | 91.107 | 1.00 | 27.85 |
| ATOM | 4620 | O   | ASP | A | 578 | 12.570 | 63.076 | 90.708 | 1.00 | 30.77 |
| ATOM | 4621 | CB  | ASP | A | 578 | 13.476 | 61.245 | 93.327 | 1.00 | 33.08 |
| ATOM | 4622 | CG  | ASP | A | 578 | 14.786 | 61.757 | 93.883 | 1.00 | 55.02 |
| ATOM | 4623 | OD1 | ASP | A | 578 | 15.756 | 62.050 | 93.182 | 1.00 | 53.04 |
| ATOM | 4624 | OD2 | ASP | A | 578 | 14.750 | 61.865 | 95.202 | 1.00 | 63.74 |
| ATOM | 4625 | N   | LYS | A | 579 | 14.804 | 62.870 | 90.966 | 1.00 | 22.71 |
| ATOM | 4626 | CA  | LYS | A | 579 | 15.127 | 64.115 | 90.359 | 1.00 | 20.47 |
| ATOM | 4627 | C   | LYS | A | 579 | 14.602 | 64.319 | 88.957 | 1.00 | 28.20 |
| ATOM | 4628 | O   | LYS | A | 579 | 14.298 | 65.451 | 88.583 | 1.00 | 31.58 |
| ATOM | 4629 | CB  | LYS | A | 579 | 16.617 | 64.350 | 90.417 | 1.00 | 22.01 |
| ATOM | 4630 | CG  | LYS | A | 579 | 17.095 | 64.370 | 91.843 | 1.00 | 35.26 |
| ATOM | 4631 | CD  | LYS | A | 579 | 17.107 | 65.791 | 92.377 | 1.00 | 60.65 |
| ATOM | 4632 | CE  | LYS | A | 579 | 16.489 | 65.928 | 93.762 | 1.00 | 72.01 |
| ATOM | 4633 | NZ  | LYS | A | 579 | 16.747 | 64.783 | 94.655 | 1.00 | 60.98 |
| ATOM | 4634 | N   | SER | A | 580 | 14.521 | 63.273 | 88.144 | 1.00 | 21.08 |
| ATOM | 4635 | CA  | SER | A | 580 | 14.055 | 63.477 | 86.749 | 1.00 | 20.19 |
| ATOM | 4636 | C   | SER | A | 580 | 12.692 | 62.922 | 86.402 | 1.00 | 23.42 |
| ATOM | 4637 | O   | SER | A | 580 | 12.270 | 63.056 | 85.257 | 1.00 | 23.98 |
| ATOM | 4638 | CB  | SER | A | 580 | 14.999 | 62.794 | 85.775 | 1.00 | 17.94 |
| ATOM | 4639 | OG  | SER | A | 580 | 15.249 | 61.485 | 86.256 | 1.00 | 16.46 |
| ATOM | 4640 | N   | HIS | A | 581 | 12.041 | 62.278 | 87.369 | 1.00 | 20.59 |
| ATOM | 4641 | CA  | HIS | A | 581 | 10.745 | 61.645 | 87.151 | 1.00 | 20.64 |
| ATOM | 4642 | C   | HIS | A | 581 | 9.685  | 62.510 | 86.446 | 1.00 | 23.45 |
| ATOM | 4643 | O   | HIS | A | 581 | 9.171  | 62.178 | 85.387 | 1.00 | 22.42 |
| ATOM | 4644 | CB  | HIS | A | 581 | 10.236 | 61.004 | 88.450 | 1.00 | 22.31 |
| ATOM | 4645 | CG  | HIS | A | 581 | 8.875  | 60.458 | 88.269 | 1.00 | 28.87 |
| ATOM | 4646 | ND1 | HIS | A | 581 | 7.755  | 61.242 | 88.508 | 1.00 | 32.80 |
| ATOM | 4647 | CD2 | HIS | A | 581 | 8.459  | 59.235 | 87.851 | 1.00 | 31.70 |
| ATOM | 4648 | CE1 | HIS | A | 581 | 6.689  | 60.483 | 88.239 | 1.00 | 32.67 |
| ATOM | 4649 | NE2 | HIS | A | 581 | 7.081  | 59.276 | 87.843 | 1.00 | 33.25 |
| ATOM | 4650 | N   | ASP | A | 582 | 9.364  | 63.646 | 87.038 | 1.00 | 19.72 |
| ATOM | 4651 | CA  | ASP | A | 582 | 8.382  | 64.520 | 86.470 | 1.00 | 21.79 |
| ATOM | 4652 | C   | ASP | A | 582 | 8.739  | 64.940 | 85.060 | 1.00 | 27.16 |
| ATOM | 4653 | O   | ASP | A | 582 | 7.897  | 64.998 | 84.144 | 1.00 | 28.34 |
| ATOM | 4654 | CB  | ASP | A | 582 | 8.193  | 65.739 | 87.407 | 1.00 | 22.66 |
| ATOM | 4655 | CG  | ASP | A | 582 | 7.617  | 65.295 | 88.714 | 1.00 | 35.28 |
| ATOM | 4656 | OD1 | ASP | A | 582 | 7.257  | 64.154 | 88.903 | 1.00 | 42.01 |
| ATOM | 4657 | OD2 | ASP | A | 582 | 7.558  | 66.227 | 89.631 | 1.00 | 44.04 |
| ATOM | 4658 | N   | GLN | A | 583 | 10.014 | 65.255 | 84.896 | 1.00 | 23.25 |
| ATOM | 4659 | CA  | GLN | A | 583 | 10.489 | 65.680 | 83.602 | 1.00 | 22.94 |
| ATOM | 4660 | C   | GLN | A | 583 | 10.398 | 64.574 | 82.561 | 1.00 | 26.53 |
| ATOM | 4661 | O   | GLN | A | 583 | 10.081 | 64.823 | 81.401 | 1.00 | 26.28 |
| ATOM | 4662 | CB  | GLN | A | 583 | 11.924 | 66.186 | 83.684 | 1.00 | 24.39 |
| ATOM | 4663 | CG  | GLN | A | 583 | 12.338 | 66.800 | 82.345 | 1.00 | 34.12 |
| ATOM | 4664 | CD  | GLN | A | 583 | 13.593 | 67.633 | 82.479 | 1.00 | 48.91 |
| ATOM | 4665 | OE1 | GLN | A | 583 | 14.375 | 67.475 | 83.428 | 1.00 | 36.93 |
| ATOM | 4666 | NE2 | GLN | A | 583 | 13.780 | 68.531 | 81.530 | 1.00 | 46.01 |
| ATOM | 4667 | N   | ALA | A | 584 | 10.709 | 63.349 | 82.975 | 1.00 | 21.00 |
| ATOM | 4668 | CA  | ALA | A | 584 | 10.651 | 62.208 | 82.070 | 1.00 | 19.24 |



|      |      |     |     |   |     |        |        |        |      |         |
|------|------|-----|-----|---|-----|--------|--------|--------|------|---------|
| ATOM | 4669 | C   | ALA | A | 584 | 9.226  | 62.047 | 81.565 | 1.00 | 23.67   |
| ATOM | 4670 | O   | ALA | A | 584 | 8.954  | 61.865 | 80.369 | 1.00 | 22.58   |
| ATOM | 4671 | CB  | ALA | A | 584 | 11.065 | 60.917 | 82.774 | 1.00 | 18.73   |
| ATOM | 4672 | N   | VAL | A | 585 | 8.294  | 62.113 | 82.511 | 1.00 | 21.42   |
| ATOM | 4673 | CA  | VAL | A | 585 | 6.890  | 61.970 | 82.136 | 1.00 | 21.62   |
| ATOM | 4674 | C   | VAL | A | 585 | 6.440  | 63.073 | 81.179 | 1.00 | 25.77   |
| ATOM | 4675 | O   | VAL | A | 585 | 5.878  | 62.863 | 80.080 | 1.00 | 23.19   |
| ATOM | 4676 | CB  | VAL | A | 585 | 6.011  | 61.832 | 83.364 | 1.00 | 22.75   |
| ATOM | 4677 | CG1 | VAL | A | 585 | 4.531  | 61.886 | 82.991 | 1.00 | 21.75   |
| ATOM | 4678 | CG2 | VAL | A | 585 | 6.333  | 60.513 | 84.039 | 1.00 | 20.15   |
| ATOM | 4679 | N   | ARG | A | 586 | 6.736  | 64.281 | 81.604 | 1.00 | 22.25   |
| ATOM | 4680 | CA  | ARG | A | 586 | 6.389  | 65.399 | 80.796 | 1.00 | 22.85   |
| ATOM | 4681 | C   | ARG | A | 586 | 7.011  | 65.340 | 79.403 | 1.00 | 21.49   |
| ATOM | 4682 | O   | ARG | A | 586 | 6.392  | 65.724 | 78.438 | 1.00 | 20.15   |
| ATOM | 4683 | CB  | ARG | A | 586 | 6.643  | 66.694 | 81.550 | 1.00 | 21.80   |
| ATOM | 4684 | CG  | ARG | A | 586 | 6.769  | 67.894 | 80.646 | 1.00 | 40.65   |
| ATOM | 4685 | CD  | ARG | A | 586 | 6.961  | 69.211 | 81.412 | 1.00 | 46.26   |
| ATOM | 4686 | NE  | ARG | A | 586 | 8.104  | 69.262 | 82.340 | 1.00 | 66.08   |
| ATOM | 4687 | CZ  | ARG | A | 586 | 8.125  | 68.752 | 83.595 | 1.00 | 77.90   |
| ATOM | 4688 | NH1 | ARG | A | 586 | 7.093  | 68.104 | 84.137 | 1.00 | 76.53   |
| ATOM | 4689 | NH2 | ARG | A | 586 | 9.213  | 68.893 | 84.340 | 1.00 | 37.12   |
| ATOM | 4690 | N   | THR | A | 587 | 8.239  | 64.868 | 79.288 | 1.00 | 18.33   |
| ATOM | 4691 | CA  | THR | A | 587 | 8.919  | 64.768 | 78.009 | 1.00 | 18.54   |
| ATOM | 4692 | C   | THR | A | 587 | 8.231  | 63.731 | 77.124 | 1.00 | 24.37   |
| ATOM | 4693 | O   | THR | A | 587 | 8.076  | 63.892 | 75.912 | 1.00 | 22.43   |
| ATOM | 4694 | CB  | THR | A | 587 | 10.392 | 64.386 | 78.216 | 1.00 | 25.90   |
| ATOM | 4695 | OG1 | THR | A | 587 | 11.009 | 65.370 | 79.004 | 1.00 | 24.10   |
| ATOM | 4696 | CG2 | THR | A | 587 | 11.145 | 64.257 | 76.897 | 1.00 | 24.64   |
| ATOM | 4697 | N   | TYR | A | 588 | 7.810  | 62.641 | 77.732 | 1.00 | 20.51   |
| ATOM | 4698 | CA  | TYR | A | 588 | 7.137  | 61.633 | 76.948 | 1.00 | 21.29   |
| ATOM | 4699 | C   | TYR | A | 588 | 5.805  | 62.178 | 76.423 | 1.00 | 25.70   |
| ATOM | 4700 | O   | TYR | A | 588 | 5.426  | 62.029 | 75.270 | 1.00 | 26.35   |
| ATOM | 4701 | CB  | TYR | A | 588 | 6.880  | 60.388 | 77.801 | 1.00 | 21.73   |
| ATOM | 4702 | CG  | TYR | A | 588 | 5.843  | 59.484 | 77.194 | 1.00 | 21.63   |
| ATOM | 4703 | CD1 | TYR | A | 588 | 6.155  | 58.679 | 76.098 | 1.00 | 23.34   |
| ATOM | 4704 | CD2 | TYR | A | 588 | 4.542  | 59.442 | 77.699 | 1.00 | 21.46   |
| ATOM | 4705 | CE1 | TYR | A | 588 | 5.200  | 57.838 | 75.519 | 1.00 | 22.02   |
| ATOM | 4706 | CE2 | TYR | A | 588 | 3.569  | 58.612 | 77.138 | 1.00 | 19.76   |
| ATOM | 4707 | CZ  | TYR | A | 588 | 3.912  | 57.809 | 76.051 | 1.00 | 22.20   |
| ATOM | 4708 | OH  | TYR | A | 588 | 2.980  | 57.006 | 75.486 | 1.00 | 24.63   |
| ATOM | 4709 | N   | GLN | A | 589 | 5.070  | 62.811 | 77.313 | 1.00 | 21.16   |
| ATOM | 4710 | CA  | GLN | A | 589 | 3.791  | 63.379 | 76.959 | 1.00 | 18.99   |
| ATOM | 4711 | C   | GLN | A | 589 | 3.932  | 64.331 | 75.796 | 1.00 | 23.96</ |



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 4727 | N   | HIS | A | 591 | 6.236  | 64.331 | 73.621 | 1.00 | 20.51 |
| ATOM | 4728 | CA  | HIS | A | 591 | 6.705  | 63.689 | 72.427 | 1.00 | 20.30 |
| ATOM | 4729 | C   | HIS | A | 591 | 5.844  | 62.634 | 71.880 | 1.00 | 20.71 |
| ATOM | 4730 | O   | HIS | A | 591 | 6.020  | 62.301 | 70.730 | 1.00 | 23.08 |
| ATOM | 4731 | CB  | HIS | A | 591 | 8.021  | 62.980 | 72.735 | 1.00 | 22.13 |
| ATOM | 4732 | CG  | HIS | A | 591 | 9.134  | 63.910 | 72.585 | 1.00 | 27.37 |
| ATOM | 4733 | ND1 | HIS | A | 591 | 9.350  | 64.905 | 73.514 | 1.00 | 32.24 |
| ATOM | 4734 | CD2 | HIS | A | 591 | 10.050 | 64.036 | 71.610 | 1.00 | 30.23 |
| ATOM | 4735 | CE1 | HIS | A | 591 | 10.394 | 65.614 | 73.093 | 1.00 | 30.35 |
| ATOM | 4736 | NE2 | HIS | A | 591 | 10.834 | 65.114 | 71.950 | 1.00 | 30.36 |
| ATOM | 4737 | N   | LYS | A | 592 | 4.981  | 62.058 | 72.690 | 1.00 | 19.93 |
| ATOM | 4738 | CA  | LYS | A | 592 | 4.222  | 60.927 | 72.217 | 1.00 | 20.77 |
| ATOM | 4739 | C   | LYS | A | 592 | 3.601  | 60.982 | 70.861 | 1.00 | 28.72 |
| ATOM | 4740 | O   | LYS | A | 592 | 3.593  | 59.977 | 70.155 | 1.00 | 27.45 |
| ATOM | 4741 | CB  | LYS | A | 592 | 3.385  | 60.231 | 73.220 | 1.00 | 20.94 |
| ATOM | 4742 | CG  | LYS | A | 592 | 2.269  | 61.119 | 73.659 | 1.00 | 26.07 |
| ATOM | 4743 | CD  | LYS | A | 592 | 1.524  | 60.461 | 74.795 | 1.00 | 37.26 |
| ATOM | 4744 | CE  | LYS | A | 592 | 0.074  | 60.869 | 74.892 | 1.00 | 41.30 |
| ATOM | 4745 | NZ  | LYS | A | 592 | -0.431 | 60.656 | 76.253 | 1.00 | 36.28 |
| ATOM | 4746 | N   | ALA | A | 593 | 3.071  | 62.155 | 70.502 | 1.00 | 25.89 |
| ATOM | 4747 | CA  | ALA | A | 593 | 2.425  | 62.314 | 69.218 | 1.00 | 21.81 |
| ATOM | 4748 | C   | ALA | A | 593 | 3.318  | 62.160 | 68.009 | 1.00 | 25.37 |
| ATOM | 4749 | O   | ALA | A | 593 | 2.861  | 61.805 | 66.945 | 1.00 | 25.18 |
| ATOM | 4750 | CB  | ALA | A | 593 | 1.750  | 63.647 | 69.131 | 1.00 | 21.84 |
| ATOM | 4751 | N   | SER | A | 594 | 4.580  | 62.455 | 68.168 | 1.00 | 23.89 |
| ATOM | 4752 | CA  | SER | A | 594 | 5.511  | 62.388 | 67.071 | 1.00 | 24.88 |
| ATOM | 4753 | C   | SER | A | 594 | 6.352  | 61.123 | 67.101 | 1.00 | 24.51 |
| ATOM | 4754 | O   | SER | A | 594 | 7.234  | 60.930 | 66.268 | 1.00 | 22.77 |
| ATOM | 4755 | CB  | SER | A | 594 | 6.416  | 63.613 | 67.130 | 1.00 | 29.32 |
| ATOM | 4756 | OG  | SER | A | 594 | 7.414  | 63.407 | 68.127 | 1.00 | 41.59 |
| ATOM | 4757 | N   | MET | A | 595 | 6.086  | 60.268 | 68.086 | 1.00 | 18.86 |
| ATOM | 4758 | CA  | MET | A | 595 | 6.833  | 59.020 | 68.227 | 1.00 | 17.56 |
| ATOM | 4759 | C   | MET | A | 595 | 6.287  | 57.889 | 67.337 | 1.00 | 25.09 |
| ATOM | 4760 | O   | MET | A | 595 | 5.191  | 57.954 | 66.773 | 1.00 | 25.50 |
| ATOM | 4761 | CB  | MET | A | 595 | 6.757  | 58.535 | 69.691 | 1.00 | 17.79 |
| ATOM | 4762 | CG  | MET | A | 595 | 7.773  | 59.190 | 70.601 | 1.00 | 20.14 |
| ATOM | 4763 | SD  | MET | A | 595 | 7.484  | 58.807 | 72.362 | 1.00 | 26.49 |
| ATOM | 4764 | CE  | MET | A | 595 | 8.038  | 57.091 | 72.509 | 1.00 | 25.07 |
| ATOM | 4765 | N   | HIS | A | 596 | 7.034  | 56.805 | 67.252 | 1.00 | 19.17 |
| ATOM | 4766 | CA  | HIS | A | 596 | 6.579  | 55.642 | 66.529 | 1.00 | 17.82 |
| ATOM | 4767 | C   | HIS | A | 596 | 5.439  | 55.071 | 67.368 | 1.00 | 21.26 |
| ATOM | 4768 | O   | HIS | A | 596 | 5.507  | 55.088 | 68.584 | 1.00 | 19.86 |
| ATOM | 4769 | CB  | HIS | A | 596 | 7.725  | 54.631 | 66.359 | 1.00 | 17.98 |
| ATOM | 4    |     |     |   |     |        |        |        |      |       |



|      |      |     |           |       |        |        |      |       |
|------|------|-----|-----------|-------|--------|--------|------|-------|
| ATOM | 4785 | O   | VAL A 598 | 5.006 | 51.250 | 71.377 | 1.00 | 19.84 |
| ATOM | 4786 | CB  | VAL A 598 | 5.183 | 49.780 | 68.314 | 1.00 | 23.28 |
| ATOM | 4787 | CG1 | VAL A 598 | 5.682 | 48.758 | 69.335 | 1.00 | 21.86 |
| ATOM | 4788 | CG2 | VAL A 598 | 4.147 | 49.166 | 67.349 | 1.00 | 21.78 |
| ATOM | 4789 | N   | THR A 599 | 6.428 | 52.147 | 69.888 | 1.00 | 18.22 |
| ATOM | 4790 | CA  | THR A 599 | 7.297 | 52.711 | 70.898 | 1.00 | 19.79 |
| ATOM | 4791 | C   | THR A 599 | 6.470 | 53.600 | 71.805 | 1.00 | 22.38 |
| ATOM | 4792 | O   | THR A 599 | 6.579 | 53.587 | 73.020 | 1.00 | 20.86 |
| ATOM | 4793 | CB  | THR A 599 | 8.373 | 53.567 | 70.223 | 1.00 | 26.72 |
| ATOM | 4794 | OG1 | THR A 599 | 9.045 | 52.824 | 69.204 | 1.00 | 25.41 |

66320-072203



|      |      |     |     |   |     |       |        |        |      |        |
|------|------|-----|-----|---|-----|-------|--------|--------|------|--------|
| ATOM | 4795 | CG2 | THR | A | 599 | 9.358 | 54.074 | 71.281 | 1.00 | 22.33  |
| ATOM | 4796 | N   | ALA | A | 600 | 5.624 | 54.399 | 71.191 | 1.00 | 19.36  |
| ATOM | 4797 | CA  | ALA | A | 600 | 4.787 | 55.270 | 71.986 | 1.00 | 19.90  |
| ATOM | 4798 | C   | ALA | A | 600 | 3.925 | 54.468 | 72.927 | 1.00 | 22.41  |
| ATOM | 4799 | O   | ALA | A | 600 | 3.777 | 54.778 | 74.119 | 1.00 | 21.96  |
| ATOM | 4800 | CB  | ALA | A | 600 | 3.947 | 56.186 | 71.118 | 1.00 | 19.84  |
| ATOM | 4801 | N   | MET | A | 601 | 3.354 | 53.399 | 72.411 | 1.00 | 19.95  |
| ATOM | 4802 | CA  | MET | A | 601 | 2.524 | 52.589 | 73.302 | 1.00 | 20.17  |
| ATOM | 4803 | C   | MET | A | 601 | 3.320 | 51.981 | 74.446 | 1.00 | 21.18  |
| ATOM | 4804 | O   | MET | A | 601 | 2.884 | 51.994 | 75.589 | 1.00 | 19.90  |
| ATOM | 4805 | CB  | MET | A | 601 | 1.791 | 51.451 | 72.582 | 1.00 | 21.67  |
| ATOM | 4806 | CG  | MET | A | 601 | 1.011 | 50.612 | 73.557 | 1.00 | 23.15  |
| ATOM | 4807 | SD  | MET | A | 601 | 1.925 | 49.137 | 74.147 | 1.00 | 28.58  |
| ATOM | 4808 | CE  | MET | A | 601 | 2.227 | 48.228 | 72.603 | 1.00 | 23.92  |
| ATOM | 4809 | N   | LEU | A | 602 | 4.490 | 51.422 | 74.122 | 1.00 | 16.35  |
| ATOM | 4810 | CA  | LEU | A | 602 | 5.338 | 50.773 | 75.139 | 1.00 | 17.71  |
| ATOM | 4811 | C   | LEU | A | 602 | 5.921 | 51.708 | 76.223 | 1.00 | 18.68  |
| ATOM | 4812 | O   | LEU | A | 602 | 5.963 | 51.362 | 77.395 | 1.00 | 21.69  |
| ATOM | 4813 | CB  | LEU | A | 602 | 6.445 | 49.876 | 74.542 | 1.00 | 16.62  |
| ATOM | 4814 | CG  | LEU | A | 602 | 5.913 | 48.704 | 73.746 | 1.00 | 22.17  |
| ATOM | 4815 | CD1 | LEU | A | 602 | 7.103 | 48.028 | 73.072 | 1.00 | 25.00  |
| ATOM | 4816 | CD2 | LEU | A | 602 | 5.239 | 47.720 | 74.697 | 1.00 | 25.74  |
| ATOM | 4817 | N   | VAL | A | 603 | 6.401 | 52.884 | 75.827 | 1.00 | 16.30  |
| ATOM | 4818 | CA  | VAL | A | 603 | 6.962 | 53.796 | 76.815 | 1.00 | 14.99  |
| ATOM | 4819 | C   | VAL | A | 603 | 5.875 | 54.264 | 77.771 | 1.00 | 19.20  |
| ATOM | 4820 | O   | VAL | A | 603 | 6.120 | 54.420 | 78.958 | 1.00 | 21.24  |
| ATOM | 4821 | CB  | VAL | A | 603 | 7.667 | 54.947 | 76.154 | 1.00 | 18.27  |
| ATOM | 4822 | CG1 | VAL | A | 603 | 8.124 | 55.941 | 77.213 | 1.00 | 18.14  |
| ATOM | 4823 | CG2 | VAL | A | 603 | 8.876 | 54.419 | 75.402 | 1.00 | 17.65  |
| ATOM | 4824 | N   | GLY | A | 604 | 4.656 | 54.452 | 77.237 | 1.00 | 17.40  |
| ATOM | 4825 | CA  | GLY | A | 604 | 3.518 | 54.878 | 78.035 | 1.00 | 17.23  |
| ATOM | 4826 | C   | GLY | A | 604 | 3.190 | 53.796 | 79.054 | 1.00 | 22.30  |
| ATOM | 4827 | O   | GLY | A | 604 | 2.836 | 54.046 | 80.209 | 1.00 | 23.93  |
| ATOM | 4828 | N   | LYS | A | 605 | 3.294 | 52.552 | 78.639 | 1.00 | 19.16  |
| ATOM | 4829 | CA  | LYS | A | 605 | 3.032 | 51.458 | 79.565 | 1.00 | 22.93  |
| ATOM | 4830 | C   | LYS | A | 605 | 4.123 | 51.454 | 80.596 | 1.00 | 23.85  |
| ATOM | 4831 | O   | LYS | A | 605 | 3.857 | 51.412 | 81.765 | 1.00 | 29.61  |
| ATOM | 4832 | CB  | LYS | A | 605 | 2.973 | 50.084 | 78.900 | 1.00 | 28.91  |
| ATOM | 4833 | CG  | LYS | A | 605 | 1.739 | 49.284 | 79.286 | 1.00 | 61.42  |
| ATOM | 4834 | CD  | LYS | A | 605 | 1.614 | 47.973 | 78.520 | 1.00 | 86.36  |
| ATOM | 4835 | CE  | LYS | A | 605 | 0.474 | 47.077 | 78.998 | 1.00 | 100.00 |
| ATOM | 4836 | NZ  | LYS | A | 605 | 0.926 | 45.803 | 79.584 | 1.00 | 96.31  |
| ATOM | 4837 | N   | ASP | A | 606 | 5.360 | 51.533 | 80.136 | 1.00 | 18.74  |
| ATOM | 4838 | CA  | ASP | A | 606 | 6.512 | 51.567 | 81.020 | 1.00 | 16.75  |
| ATOM | 4839 | C   | ASP | A | 606 | 6.417 | 52.687 | 82.021 | 1.00 | 21.50  |
| ATOM | 4840 | O   | ASP | A | 606 | 6.744 | 52.500 | 83.171 | 1.00 | 23.69  |
| ATOM | 4841 | CB  | ASP | A | 606 | 7.828 | 51.737 | 80.241 | 1.00 | 18.62  |
| ATOM | 4842 | CG  | ASP | A | 606 | 8.194 | 50.551 | 79.363 | 1.00 | 33.79  |
| ATOM | 4843 | OD1 | ASP | A | 606 | 7.867 | 49.391 | 79.604 | 1.00 | 33.52  |
| ATOM | 4844 | OD2 | ASP | A | 606 | 8.916 | 50.897 | 78.323 | 1.00 | 27.00  |
| ATOM | 4845 | N   | LEU | A | 607 | 5.964 | 53.846 | 81.570 | 1.00 | 19.12  |
| ATOM | 4846 | CA  | LEU | A | 607 | 5.846 | 55.031 | 82.403 | 1.00 | 21.90  |
| ATOM | 4847 | C   | LEU | A | 607 | 4.550 | 55.057 | 83.169 | 1.00 | 28.88  |
| ATOM | 4848 | O   | LEU | A | 607 | 4.336 | 55.922 | 84.027 | 1.00 | 26.52  |
| ATOM | 4849 | CB  | LEU | A | 607 | 5.939 | 56.303 | 81.538 | 1.00 | 22.98  |
| ATOM | 4850 | CG  | LEU | A | 607 | 7.314 | 56.996 | 81.567 | 1.00 | 28.58  |
| ATOM | 4851 | CD1 | LEU | A | 607 | 8.412 | 56.004 | 81.849 | 1.00 | 31.86  |
| ATOM | 4852 | CD2 | LEU | A | 607 | 7.582 | 57.761 | 80.274 | 1.00 | 23.84  |



|      |      |      |     |   |     |         |        |        |      |        |
|------|------|------|-----|---|-----|---------|--------|--------|------|--------|
| ATOM | 4853 | N    | LYS | A | 608 | 3.673   | 54.121 | 82.823 | 1.00 | 25.73  |
| ATOM | 4854 | CA   | LYS | A | 608 | 2.402   | 54.050 | 83.483 | 1.00 | 27.14  |
| ATOM | 4855 | C    | LYS | A | 608 | 1.517   | 55.274 | 83.248 | 1.00 | 36.18  |
| ATOM | 4856 | O    | LYS | A | 608 | 0.808   | 55.735 | 84.155 | 1.00 | 36.45  |
| ATOM | 4857 | CB   | LYS | A | 608 | 2.619   | 53.872 | 84.965 | 1.00 | 28.04  |
| ATOM | 4858 | CG   | LYS | A | 608 | 3.024   | 52.458 | 85.321 | 1.00 | 34.92  |
| ATOM | 4859 | CD   | LYS | A | 608 | 3.455   | 52.351 | 86.775 | 1.00 | 62.54  |
| ATOM | 4860 | CE   | LYS | A | 608 | 4.872   | 52.865 | 87.017 | 1.00 | 100.00 |
| ATOM | 4861 | NZ   | LYS | A | 608 | 5.308   | 52.782 | 88.423 | 1.00 | 100.00 |
| ATOM | 4862 | N    | VAL | A | 609 | 1.538   | 55.817 | 82.037 | 1.00 | 33.96  |
| ATOM | 4863 | CA   | VAL | A | 609 | 0.700   | 56.960 | 81.756 | 1.00 | 35.62  |
| ATOM | 4864 | C    | VAL | A | 609 | -0.596  | 56.539 | 81.068 | 1.00 | 50.35  |
| ATOM | 4865 | O    | VAL | A | 609 | -0.570  | 55.732 | 80.140 | 1.00 | 50.27  |
| ATOM | 4866 | CB   | VAL | A | 609 | 1.399   | 58.066 | 81.015 | 1.00 | 37.98  |
| ATOM | 4867 | CG1  | VAL | A | 609 | 2.835   | 58.174 | 81.464 | 1.00 | 36.77  |
| ATOM | 4868 | CG2  | VAL | A | 609 | 1.344   | 57.776 | 79.539 | 1.00 | 40.19  |
| ATOM | 4869 | N    | ASP | A | 610 | -1.725  | 57.084 | 81.569 | 1.00 | 53.33  |
| ATOM | 4870 | CA   | ASP | A | 610 | -3.086  | 56.822 | 81.095 | 1.00 | 89.47  |
| ATOM | 4871 | C    | ASP | A | 610 | -3.734  | 55.681 | 81.880 | 1.00 | 100.00 |
| ATOM | 4872 | O    | ASP | A | 610 | -4.010  | 55.789 | 83.081 | 1.00 | 67.46  |
| ATOM | 4873 | CB   | ASP | A | 610 | -3.181  | 56.608 | 79.571 | 1.00 | 91.20  |
| ATOM | 4874 | CG   | ASP | A | 610 | -3.263  | 57.902 | 78.800 | 1.00 | 99.31  |
| ATOM | 4875 | OD1  | ASP | A | 610 | -4.214  | 58.659 | 78.852 | 1.00 | 100.00 |
| ATOM | 4876 | OD2  | ASP | A | 610 | -2.208  | 58.121 | 78.053 | 1.00 | 99.03  |
| ATOM | 4877 | ZN2+ | ZN  | Z | 1   | 16.867  | 38.938 | 64.588 | 1.00 | 19.85  |
| ATOM | 4878 | YB3+ | YB  | Y | 1   | 42.592  | 51.139 | 99.562 | 1.00 | 19.75  |
| ATOM | 4879 | YB3+ | YB  | Y | 2   | -13.987 | 57.035 | 52.274 | 0.50 | 30.89  |
| ATOM | 4880 | YB3+ | YB  | Y | 3   | -10.598 | 57.976 | 52.424 | 0.50 | 22.65  |
| ATOM | 4881 | CG   | IMD | I | 1   | 25.977  | 42.326 | 80.640 | 1.00 | 21.27  |
| ATOM | 4882 | ND1  | IMD | I | 1   | 25.984  | 42.381 | 79.258 | 1.00 | 26.76  |
| ATOM | 4883 | CD2  | IMD | I | 1   | 27.243  | 42.000 | 81.012 | 1.00 | 18.44  |
| ATOM | 4884 | CE1  | IMD | I | 1   | 27.198  | 42.109 | 78.814 | 1.00 | 23.26  |
| ATOM | 4885 | NE2  | IMD | I | 1   | 27.978  | 41.865 | 79.858 | 1.00 | 31.16  |
| ATOM | 4886 | CB   | ACE | C | 1   | 13.682  | 11.710 | 69.377 | 1.00 | 100.00 |
| ATOM | 4887 | CG   | ACE | C | 1   | 12.730  | 12.944 | 69.296 | 1.00 | 100.00 |
| ATOM | 4888 | OD2  | ACE | C | 1   | 11.957  | 12.700 | 70.111 | 1.00 | 28.08  |
| ATOM | 4889 | OD1  | ACE | C | 1   | 13.221  | 14.170 | 69.327 | 1.00 | 29.42  |
| ATOM | 4890 | C4   | HA1 | H | 1   | 7.929   | 39.787 | 68.124 | 1.00 | 33.98  |
| ATOM | 4891 | C3   | HA1 | H | 1   | 7.915   | 38.456 | 67.710 | 1.00 | 34.29  |
| ATOM | 4892 | C2   | HA1 | H | 1   | 7.854   | 37.393 | 68.601 | 1.00 | 27.23  |
| ATOM | 4893 | C1   | HA1 | H | 1   | 7.750   | 37.660 | 69.963 | 1.00 | 31.46  |
| ATOM | 4894 | C6   | HA1 | H | 1   | 7.662   | 38.984 | 70.398 | 1.00 | 31.55  |
| ATOM | 4895 | C5   | HA1 | H | 1   | 7.795   | 40.040 | 69.485 | 1.00 | 28.1   |



|      |      |     |     |   |    |         |        |         |      |       |
|------|------|-----|-----|---|----|---------|--------|---------|------|-------|
| ATOM | 4911 | O3  | HA1 | H | 1  | 17.468  | 43.810 | 64.424  | 1.00 | 32.19 |
| ATOM | 4912 | C18 | HA1 | H | 1  | 18.102  | 42.561 | 66.330  | 1.00 | 41.82 |
| ATOM | 4913 | C19 | HA1 | H | 1  | 17.414  | 43.354 | 67.436  | 1.00 | 55.81 |
| ATOM | 4914 | C20 | HA1 | H | 1  | 18.370  | 43.767 | 68.541  | 1.00 | 63.54 |
| ATOM | 4915 | C21 | HA1 | H | 1  | 17.851  | 44.929 | 69.366  | 1.00 | 62.49 |
| ATOM | 4916 | C22 | HA1 | H | 1  | 17.521  | 46.129 | 68.497  | 1.00 | 56.55 |
| ATOM | 4917 | O4  | HA1 | H | 1  | 16.627  | 46.104 | 67.664  | 1.00 | 64.73 |
| ATOM | 4918 | O5  | HA1 | H | 1  | 18.077  | 47.221 | 68.942  | 1.00 | 39.37 |
| ATOM | 4919 | O   | HOH | W | 1  | 23.566  | 34.022 | 75.376  | 1.00 | 12.30 |
| ATOM | 4920 | O   | HOH | W | 2  | 13.388  | 27.777 | 78.688  | 1.00 | 13.34 |
| ATOM | 4921 | O   | HOH | W | 3  | 25.835  | 18.549 | 79.662  | 1.00 | 27.10 |
| ATOM | 4922 | O   | HOH | W | 4  | 25.597  | 20.037 | 56.101  | 1.00 | 31.91 |
| ATOM | 4923 | O   | HOH | W | 5  | 10.677  | 54.449 | 68.009  | 1.00 | 18.65 |
| ATOM | 4924 | O   | HOH | W | 6  | -10.132 | 46.969 | 60.385  | 1.00 | 32.14 |
| ATOM | 4925 | O   | HOH | W | 7  | 2.593   | 37.637 | 61.650  | 1.00 | 21.00 |
| ATOM | 4926 | O   | HOH | W | 8  | -7.181  | 40.515 | 62.968  | 1.00 | 27.33 |
| ATOM | 4927 | O   | HOH | W | 9  | 43.698  | 44.858 | 76.466  | 1.00 | 45.00 |
| ATOM | 4928 | O   | HOH | W | 10 | 15.570  | 28.918 | 62.416  | 1.00 | 21.48 |
| ATOM | 4929 | O   | HOH | W | 11 | -1.589  | 36.832 | 71.268  | 1.00 | 30.40 |
| ATOM | 4930 | O   | HOH | W | 12 | -2.055  | 28.558 | 60.781  | 1.00 | 22.31 |
| ATOM | 4931 | O   | HOH | W | 13 | 20.676  | 44.343 | 79.098  | 1.00 | 32.97 |
| ATOM | 4932 | O   | HOH | W | 14 | 3.431   | 26.421 | 58.090  | 1.00 | 45.38 |
| ATOM | 4933 | O   | HOH | W | 15 | -4.614  | 50.837 | 59.260  | 1.00 | 25.79 |
| ATOM | 4934 | O   | HOH | W | 16 | 36.272  | 36.591 | 76.038  | 1.00 | 17.59 |
| ATOM | 4935 | O   | HOH | W | 17 | 32.654  | 39.309 | 77.187  | 1.00 | 23.80 |
| ATOM | 4936 | O   | HOH | W | 18 | 17.065  | 55.043 | 87.500  | 1.00 | 25.70 |
| ATOM | 4937 | O   | HOH | W | 19 | 40.120  | 54.721 | 100.891 | 1.00 | 17.97 |
| ATOM | 4938 | O   | HOH | W | 20 | 24.948  | 56.731 | 93.762  | 1.00 | 23.67 |
| ATOM | 4939 | O   | HOH | W | 21 | 5.307   | 31.463 | 78.439  | 1.00 | 25.94 |
| ATOM | 4940 | O   | HOH | W | 22 | 29.601  | 35.642 | 82.806  | 1.00 | 25.64 |
| ATOM | 4941 | O   | HOH | W | 23 | 42.458  | 58.650 | 95.509  | 1.00 | 26.81 |
| ATOM | 4942 | O   | HOH | W | 24 | 41.450  | 41.107 | 78.272  | 1.00 | 24.09 |
| ATOM | 4943 | O   | HOH | W | 25 | 22.573  | 45.711 | 84.050  | 1.00 | 19.66 |
| ATOM | 4944 | O   | HOH | W | 26 | 6.739   | 45.508 | 66.460  | 1.00 | 24.65 |
| ATOM | 4945 | O   | HOH | W | 27 | 17.394  | 39.743 | 52.082  | 1.00 | 23.53 |
| ATOM | 4946 | O   | HOH | W | 28 | 24.544  | 45.460 | 82.019  | 1.00 | 16.68 |
| ATOM | 4947 | O   | HOH | W | 29 | 24.772  | 68.201 | 81.705  | 1.00 | 33.19 |
| ATOM | 4948 | O   | HOH | W | 30 | 1.837   | 33.333 | 67.260  | 1.00 | 21.31 |
| ATOM | 4949 | O   | HOH | W | 31 | 4.415   | 69.786 | 58.410  | 1.00 | 35.00 |
| ATOM | 4950 | O   | HOH | W | 32 | 7.455   | 46.261 | 57.394  | 1.00 | 25.67 |
| ATOM | 4951 | O   | HOH | W | 33 | -9.584  | 46.880 | 63.997  | 1.00 | 24.93 |
| ATOM | 4952 | O   | HOH | W | 34 | -3.024  | 25.330 | 60.767  | 1.00 | 42.66 |
| ATOM | 4953 | O   | HOH | W | 35 | 17.847  | 39.318 | 55.530  | 1.00 | 23.09 |
| ATOM | 4954 | O   | HOH | W | 36 | 23.296  | 70.064 | 87.984  | 1.00 | 42.74 |
| ATOM | 4955 | O   | HOH | W | 37 | 32.919  | 53.636 | 68.454  | 1.00 | 26.30 |
| ATOM | 4956 | O   | HOH | W | 38 | 29.879  | 45.644 | 50.852  | 1.00 | 30.86 |
| ATOM | 4957 | O   | HOH | W | 39 | 10.807  | 31.399 | 52.856  | 1.00 | 22.94 |
| ATOM | 4958 | O   | HOH | W | 40 | 31.341  | 28.804 | 81.757  | 1.00 | 27.83 |
| ATOM | 4959 | O   | HOH | W | 41 | 19.787  | 60.946 | 66.660  | 1.00 | 34.61 |
| ATOM | 4960 | O   | HOH | W | 42 | 5.475   | 60.634 | 63.442  | 1.00 | 23.64 |
| ATOM | 4961 | O   | HOH | W | 43 | 37.820  | 49.977 | 69.049  | 1.00 | 34.63 |
| ATOM | 4962 | O   | HOH | W | 44 | 8.776   | 45.288 | 71.439  | 1.00 | 24.05 |
| ATOM | 4963 | O   | HOH | W | 45 | 45.482  | 56.302 | 77.061  | 1.00 | 55.80 |
| ATOM | 4964 | O   | HOH | W | 46 | 33.235  | 31.270 | 62.597  | 1.00 | 31.95 |
| ATOM | 4965 | O   | HOH | W | 47 | -1.953  | 55.133 | 57.155  | 1.00 | 21.83 |
| ATOM | 4966 | O   | HOH | W | 48 | 26.604  | 54.881 | 67.253  | 1.00 | 20.30 |
| ATOM | 4967 | O   | HOH | W | 49 | 14.297  | 66.865 | 85.395  | 1.00 | 31.63 |
| ATOM | 4968 | O   | HOH | W | 50 | 7.263   | 47.979 | 65.596  | 1.00 | 37.56 |



|      |      |   |     |   |    |         |        |        |      |       |
|------|------|---|-----|---|----|---------|--------|--------|------|-------|
| ATOM | 4969 | O | HOH | W | 51 | 37.920  | 36.114 | 73.995 | 1.00 | 14.86 |
| ATOM | 4970 | O | HOH | W | 52 | 28.377  | 48.590 | 61.079 | 1.00 | 37.27 |
| ATOM | 4971 | O | HOH | W | 53 | 2.116   | 28.905 | 53.079 | 1.00 | 42.56 |
| ATOM | 4972 | O | HOH | W | 54 | 35.521  | 22.458 | 64.953 | 1.00 | 26.17 |
| ATOM | 4973 | O | HOH | W | 55 | 7.851   | 19.910 | 84.778 | 1.00 | 22.04 |
| ATOM | 4974 | O | HOH | W | 56 | -14.352 | 49.917 | 56.200 | 1.00 | 34.62 |
| ATOM | 4975 | O | HOH | W | 57 | 26.924  | 39.331 | 68.855 | 1.00 | 24.29 |
| ATOM | 4976 | O | HOH | W | 58 | 16.076  | 27.261 | 80.879 | 1.00 | 21.38 |
| ATOM | 4977 | O | HOH | W | 59 | 29.747  | 44.590 | 66.215 | 1.00 | 37.34 |
| ATOM | 4978 | O | HOH | W | 60 | 29.210  | 23.547 | 77.093 | 1.00 | 31.98 |
| ATOM | 4979 | O | HOH | W | 61 | 28.910  | 50.667 | 63.027 | 1.00 | 22.20 |
| ATOM | 4980 | O | HOH | W | 62 | 20.042  | 19.974 | 84.146 | 1.00 | 31.02 |
| ATOM | 4981 | O | HOH | W | 63 | 20.576  | 35.333 | 45.069 | 1.00 | 26.25 |
| ATOM | 4982 | O | HOH | W | 64 | -0.215  | 29.800 | 72.342 | 1.00 | 33.17 |
| ATOM | 4983 | O | HOH | W | 65 | -1.089  | 45.685 | 73.734 | 1.00 | 33.57 |
| ATOM | 4984 | O | HOH | W | 66 | 0.438   | 52.886 | 76.077 | 1.00 | 32.51 |
| ATOM | 4985 | O | HOH | W | 67 | 14.167  | 74.815 | 49.997 | 1.00 | 17.05 |
| ATOM | 4986 | O | HOH | W | 68 | -4.646  | 34.746 | 72.149 | 1.00 | 26.96 |
| ATOM | 4987 | O | HOH | W | 69 | -0.608  | 33.321 | 77.691 | 1.00 | 28.42 |
| ATOM | 4988 | O | HOH | W | 70 | 44.174  | 49.671 | 78.015 | 1.00 | 44.09 |
| ATOM | 4989 | O | HOH | W | 71 | 18.342  | 56.463 | 89.617 | 1.00 | 24.87 |
| ATOM | 4990 | O | HOH | W | 72 | -3.402  | 50.274 | 64.069 | 1.00 | 32.32 |
| ATOM | 4991 | O | HOH | W | 73 | 35.472  | 42.694 | 55.658 | 1.00 | 29.12 |
| ATOM | 4992 | O | HOH | W | 74 | 39.633  | 49.627 | 92.786 | 1.00 | 23.74 |
| ATOM | 4993 | O | HOH | W | 75 | 23.814  | 44.857 | 73.613 | 1.00 | 36.27 |
| ATOM | 4994 | O | HOH | W | 76 | 4.137   | 65.690 | 43.494 | 1.00 | 41.73 |
| ATOM | 4995 | O | HOH | W | 77 | -2.873  | 36.499 | 53.879 | 1.00 | 32.19 |
| ATOM | 4996 | O | HOH | W | 78 | 19.723  | 36.789 | 86.029 | 1.00 | 23.01 |
| ATOM | 4997 | O | HOH | W | 79 | 32.756  | 42.684 | 86.988 | 1.00 | 26.34 |
| ATOM | 4998 | O | HOH | W | 80 | -13.494 | 53.592 | 58.883 | 1.00 | 48.04 |
| ATOM | 4999 | O | HOH | W | 81 | 10.287  | 35.426 | 76.025 | 1.00 | 42.73 |
| ATOM | 5000 | O | HOH | W | 82 | 11.794  | 38.320 | 43.226 | 1.00 | 38.16 |
| ATOM | 5001 | O | HOH | W | 83 | 12.911  | 64.532 | 53.870 | 1.00 | 32.51 |
| ATOM | 5002 | O | HOH | W | 84 | 23.737  | 48.333 | 68.074 | 1.00 | 20.34 |
| ATOM | 5003 | O | HOH | W | 85 | 10.259  | 47.114 | 58.559 | 1.00 | 25.59 |
| ATOM | 5004 | O | HOH | W | 86 | 10.648  | 53.408 | 86.123 | 1.00 | 28.02 |
| ATOM | 5005 | O | HOH | W | 87 | 6.095   | 34.678 | 88.868 | 1.00 | 27.11 |
| ATOM | 5006 | O | HOH | W | 88 | 10.406  | 35.822 | 89.126 | 1.00 | 37.02 |
| ATOM | 5007 | O | HOH | W | 89 | 45.214  | 48.270 | 89.083 | 1.00 | 41.53 |
| ATOM | 5008 | O | HOH | W | 90 | 1.875   | 28.252 | 68.827 | 1.00 | 32.79 |
| ATOM | 5009 | O | HOH | W | 91 | 20.183  | 28.258 | 51.122 | 1.00 | 37.70 |
| ATOM | 5010 | O | HOH | W | 92 | 39.933  | 60.917 | 79.130 | 1.00 | 29.50 |
| ATOM | 5011 | O | HOH | W | 93 | 10.589  | 68.582 | 87.108 |      |       |



|      |      |   |       |   |     |         |        |         |      |       |
|------|------|---|-------|---|-----|---------|--------|---------|------|-------|
| ATOM | 5027 | O | HOH   | W | 109 | 37.414  | 53.648 | 66.810  | 1.00 | 62.05 |
| ATOM | 5028 | O | HOH   | W | 110 | -9.983  | 46.517 | 74.286  | 1.00 | 52.15 |
| ATOM | 5029 | O | HOH   | W | 111 | 28.275  | 66.451 | 78.187  | 1.00 | 20.97 |
| ATOM | 5030 | O | HOH   | W | 112 | 0.299   | 38.957 | 40.503  | 1.00 | 50.56 |
| ATOM | 5031 | O | HOH   | W | 113 | 5.444   | 44.057 | 39.458  | 1.00 | 52.33 |
| ATOM | 5032 | O | HOH   | W | 114 | 30.644  | 32.062 | 49.915  | 1.00 | 36.21 |
| ATOM | 5033 | O | HOH   | W | 115 | 18.252  | 26.342 | 50.525  | 1.00 | 45.23 |
| ATOM | 5034 | O | HOH   | W | 116 | 13.526  | 15.084 | 61.080  | 1.00 | 37.70 |
| ATOM | 5035 | O | HOH   | W | 117 | -13.979 | 18.969 | 42.299  | 1.00 | 56.22 |
| ATOM | 5036 | O | HOH   | W | 118 | 26.776  | 25.413 | 84.339  | 1.00 | 35.77 |
| ATOM | 5037 | O | HOH   | W | 119 | 11.930  | 58.269 | 71.061  | 1.00 | 23.92 |
| ATOM | 5038 | O | HOH   | W | 120 | 34.912  | 67.869 | 86.385  | 1.00 | 24.32 |
| ATOM | 5039 | O | HOH   | W | 121 | 24.502  | 71.580 | 83.464  | 1.00 | 30.05 |
| ATOM | 5040 | O | HOH   | W | 122 | 25.720  | 67.144 | 90.575  | 1.00 | 33.20 |
| ATOM | 5041 | O | HOH   | W | 123 | 27.913  | 32.926 | 85.600  | 1.00 | 40.23 |
| ATOM | 5042 | O | HOH   | W | 124 | 34.782  | 68.339 | 71.280  | 1.00 | 36.93 |
| ATOM | 5043 | O | HOH   | W | 125 | 15.535  | 41.733 | 77.570  | 1.00 | 43.41 |
| ATOM | 5044 | O | HOH   | W | 126 | 39.295  | 44.865 | 92.155  | 1.00 | 38.08 |
| ATOM | 5045 | O | HOH   | W | 127 | 34.644  | 38.435 | 88.608  | 1.00 | 43.36 |
| ATOM | 5046 | O | HOH   | W | 128 | 16.902  | 68.175 | 82.059  | 1.00 | 33.39 |
| ATOM | 5047 | O | HOH   | W | 129 | 23.092  | 69.396 | 79.614  | 1.00 | 43.52 |
| ATOM | 5048 | O | HOH   | W | 130 | 38.423  | 66.837 | 74.075  | 1.00 | 44.21 |
| ATOM | 5049 | O | HOH   | W | 131 | 20.725  | 15.554 | 56.723  | 1.00 | 58.73 |
| ATOM | 5050 | O | HOH   | W | 132 | 10.791  | 73.362 | 50.162  | 1.00 | 53.71 |
| ATOM | 5051 | O | HOH   | W | 133 | 34.794  | 62.523 | 92.372  | 1.00 | 44.50 |
| ATOM | 5052 | O | HOH   | W | 134 | 44.478  | 50.279 | 84.427  | 1.00 | 43.68 |
| ATOM | 5053 | O | HOH   | W | 135 | 34.311  | 29.805 | 80.713  | 1.00 | 45.96 |
| ATOM | 5054 | O | HOH   | W | 136 | 40.841  | 39.740 | 89.975  | 1.00 | 60.88 |
| ATOM | 5055 | O | HOH   | W | 137 | 25.356  | 40.542 | 42.066  | 1.00 | 41.02 |
| ATOM | 5056 | O | HOH   | W | 138 | 28.438  | 44.085 | 75.926  | 1.00 | 41.72 |
| ATOM | 5057 | O | HOH   | W | 139 | 25.711  | 38.832 | 88.780  | 1.00 | 65.21 |
| ATOM | 5058 | O | HOH   | W | 140 | 11.923  | 76.777 | 49.321  | 1.00 | 58.57 |
| ATOM | 5059 | O | HOH   | W | 141 | 24.266  | 34.539 | 87.344  | 1.00 | 50.29 |
| ATOM | 5060 | O | HOH   | W | 142 | 16.030  | 9.532  | 72.041  | 1.00 | 48.71 |
| ATOM | 5061 | O | HOH   | W | 143 | -3.177  | 67.341 | 56.141  | 1.00 | 42.73 |
| ATOM | 5062 | O | HOH   | W | 144 | 50.825  | 56.903 | 100.142 | 1.00 | 59.75 |
| ATOM | 5063 | O | HOH   | W | 145 | 0.820   | 71.358 | 71.084  | 1.00 | 40.87 |
| ATOM | 5064 | O | HOH   | W | 146 | -17.608 | 36.729 | 42.417  | 1.00 | 45.50 |
| ATOM | 5065 | O | HOH   | W | 147 | 28.308  | 19.679 | 78.841  | 1.00 | 36.05 |
| ATOM | 5066 | O | HOH   | W | 148 | 2.463   | 58.104 | 67.862  | 1.00 | 44.11 |
| ATOM | 5067 | O | HOH   | W | 149 | 10.592  | 23.631 | 48.575  | 1.00 | 63.18 |
| ATOM | 5068 | O | HOH   | W | 150 | 6.654   | 22.341 | 57.393  | 1.00 | 46.55 |
| ATOM | 5069 | O | HOH</ |   |     |         |        |         |      |       |



00320-000000

|      |      |   |           |         |        |         |      |       |
|------|------|---|-----------|---------|--------|---------|------|-------|
| ATOM | 5085 | O | HOH W 167 | -7.109  | 31.913 | 64.267  | 1.00 | 60.17 |
| ATOM | 5086 | O | HOH W 168 | 13.620  | 57.052 | 40.950  | 1.00 | 50.59 |
| ATOM | 5087 | O | HOH W 169 | 24.100  | 13.750 | 57.699  | 1.00 | 57.30 |
| ATOM | 5088 | O | HOH W 170 | -1.060  | 50.178 | 39.555  | 1.00 | 53.44 |
| ATOM | 5089 | O | HOH W 171 | 28.136  | 38.840 | 82.951  | 1.00 | 65.23 |
| ATOM | 5090 | O | HOH W 172 | 33.383  | 46.065 | 62.179  | 1.00 | 54.17 |
| ATOM | 5091 | O | HOH W 173 | 32.676  | 64.388 | 94.464  | 1.00 | 63.25 |
| ATOM | 5092 | O | HOH W 174 | 28.895  | 34.922 | 43.046  | 1.00 | 65.00 |
| ATOM | 5093 | O | HOH W 175 | 1.150   | 50.642 | 82.686  | 1.00 | 50.19 |
| ATOM | 5094 | O | HOH W 176 | 38.269  | 37.461 | 84.426  | 1.00 | 55.97 |
| ATOM | 5095 | O | HOH W 177 | 28.133  | 15.115 | 62.115  | 1.00 | 54.46 |
| ATOM | 5096 | O | HOH W 178 | -21.180 | 27.797 | 43.644  | 1.00 | 41.51 |
| ATOM | 5097 | O | HOH W 179 | 37.216  | 39.040 | 89.229  | 1.00 | 51.67 |
| ATOM | 5098 | O | HOH W 180 | -16.439 | 50.762 | 42.943  | 1.00 | 52.31 |
| ATOM | 5099 | O | HOH W 181 | 27.532  | 70.756 | 92.817  | 1.00 | 51.38 |
| ATOM | 5100 | O | HOH W 182 | 17.249  | 54.147 | 94.044  | 1.00 | 60.50 |
| ATOM | 5101 | O | HOH W 183 | 30.255  | 42.249 | 74.632  | 1.00 | 59.08 |
| ATOM | 5102 | O | HOH W 184 | 7.869   | 71.095 | 47.756  | 1.00 | 47.99 |
| ATOM | 5103 | O | HOH W 185 | -3.927  | 35.976 | 39.455  | 1.00 | 54.08 |
| ATOM | 5104 | O | HOH W 186 | 17.648  | 48.041 | 85.644  | 1.00 | 48.63 |
| ATOM | 5105 | O | HOH W 187 | 16.843  | 63.121 | 61.640  | 1.00 | 55.70 |
| ATOM | 5106 | O | HOH W 188 | 32.678  | 67.498 | 91.570  | 1.00 | 46.01 |
| ATOM | 5107 | O | HOH W 189 | 26.777  | 67.291 | 92.968  | 1.00 | 62.50 |
| ATOM | 5108 | O | HOH W 190 | 43.626  | 47.465 | 93.713  | 1.00 | 48.48 |
| ATOM | 5109 | O | HOH W 191 | 19.866  | 63.522 | 93.923  | 1.00 | 49.85 |
| ATOM | 5110 | O | HOH W 192 | 31.772  | 43.653 | 64.750  | 1.00 | 61.07 |
| ATOM | 5111 | O | HOH W 193 | 15.157  | 75.463 | 53.328  | 1.00 | 32.84 |
| ATOM | 5112 | O | HOH W 194 | 34.792  | 45.584 | 97.991  | 1.00 | 58.67 |
| ATOM | 5113 | O | HOH W 195 | 37.064  | 21.576 | 67.060  | 1.00 | 54.68 |
| ATOM | 5114 | O | HOH W 196 | 30.070  | 14.758 | 70.646  | 1.00 | 51.43 |
| ATOM | 5115 | O | HOH W 197 | 28.860  | 72.257 | 75.634  | 1.00 | 62.52 |
| ATOM | 5116 | O | HOH W 198 | 8.471   | 19.419 | 57.691  | 1.00 | 57.63 |
| ATOM | 5117 | O | HOH W 199 | 0.503   | 41.546 | 78.765  | 1.00 | 56.21 |
| ATOM | 5118 | O | HOH W 200 | 50.521  | 54.089 | 79.412  | 1.00 | 51.01 |
| ATOM | 5119 | O | HOH W 201 | -0.543  | 52.686 | 81.009  | 1.00 | 46.93 |
| ATOM | 5120 | O | HOH W 202 | 26.682  | 58.450 | 96.254  | 1.00 | 50.09 |
| ATOM | 5121 | O | HOH W 203 | 17.549  | 42.811 | 71.646  | 1.00 | 57.91 |
| ATOM | 5122 | O | HOH W 204 | 29.750  | 18.123 | 58.438  | 1.00 | 66.60 |
| ATOM | 5123 | O | HOH W 205 | 22.570  | 40.343 | 42.345  | 1.00 | 59.88 |
| ATOM | 5124 | O | HOH W 206 | -13.013 | 21.974 | 59.037  | 1.00 | 67.74 |
| ATOM | 5125 | O | HOH W 207 | 1.213   | 62.922 | 83.165  | 1.00 | 62.70 |
| ATOM | 5126 | O | HOH W 208 | 3.178   | 70.030 | 60.833  | 1.00 | 48.41 |
| ATOM | 5127 | O | HOH W 209 | 35.803  | 16.258 | 65.017  | 1.00 | 58.97 |
| ATOM | 5128 | O | HOH W 210 | 46.693  | 53.513 | 105.644 | 1.00 | 53.44 |
| ATOM | 5129 | O | HOH W 211 | 4.942   | 70.389 | 45.132  | 1.00 | 53.10 |
| ATOM | 5130 | O | HOH W 212 | 37.457  | 25.190 | 67.060  | 1.00 | 63.53 |
| ATOM | 5131 | O | HOH W 213 | 11.196  | 29.803 | 45.434  | 1.00 | 53.63 |
| ATOM | 5132 | O | HOH W 214 | 26.923  | 61.460 | 54.700  | 1.00 | 69.19 |
| ATOM | 5133 | O | HOH W 215 | 0.546   | 69.044 | 72.439  | 1.00 | 39.60 |
| ATOM | 5134 | O | HOH W 216 | -23.701 | 40.796 | 47.831  | 1.00 | 52.83 |
| ATOM | 5135 | O | HOH W 217 | 12.204  | 39.839 | 90.814  | 1.00 | 47.33 |
| ATOM | 5136 | O | HOH W 218 | 33.128  | 42.150 | 94.157  | 1.00 | 56.23 |
| ATOM | 5137 | O | HOH W 219 | 49.923  | 57.382 | 98.346  | 1.00 | 58.39 |
| ATOM | 5138 | O | HOH W 220 | 32.977  | 13.997 | 66.958  | 1.00 | 60.97 |
| ATOM | 5139 | O | HOH W 221 | 20.874  | 69.427 | 54.701  | 1.00 | 55.56 |
| ATOM | 5140 | O | HOH W 223 | -19.866 | 36.630 | 55.598  | 1.00 | 56.17 |
| ATOM | 5141 | O | HOH W 224 | 38.826  | 44.981 | 56.301  | 1.00 | 57.17 |
| ATOM | 5142 | O | HOH W 225 | 18.003  | 44.053 | 79.512  | 1.00 | 56.10 |



|      |      |   |     |   |     |         |        |        |      |       |
|------|------|---|-----|---|-----|---------|--------|--------|------|-------|
| ATOM | 5143 | O | HOH | W | 226 | 6.358   | 21.380 | 58.894 | 1.00 | 66.63 |
| ATOM | 5144 | O | HOH | W | 227 | 29.345  | 15.953 | 82.008 | 1.00 | 60.35 |
| ATOM | 5145 | O | HOH | W | 228 | -18.860 | 45.061 | 58.589 | 1.00 | 60.74 |
| ATOM | 5146 | O | HOH | W | 229 | -17.851 | 43.055 | 49.022 | 1.00 | 52.29 |
| ATOM | 5147 | O | HOH | W | 230 | -0.184  | 59.399 | 61.998 | 1.00 | 45.48 |
| ATOM | 5148 | O | HOH | W | 231 | 16.645  | 54.043 | 90.579 | 1.00 | 63.17 |
| ATOM | 5149 | O | HOH | W | 232 | 7.766   | 63.225 | 91.375 | 1.00 | 63.27 |
| ATOM | 5150 | O | HOH | W | 233 | 26.321  | 54.492 | 43.345 | 1.00 | 53.24 |
| ATOM | 5151 | O | HOH | W | 234 | 25.867  | 54.044 | 96.258 | 1.00 | 59.57 |
| ATOM | 5152 | O | HOH | W | 235 | 23.499  | 50.875 | 40.953 | 1.00 | 68.77 |
| ATOM | 5153 | O | HOH | W | 236 | -5.445  | 53.893 | 45.137 | 1.00 | 54.78 |
| ATOM | 5154 | O | HOH | W | 237 | 17.844  | 70.747 | 82.442 | 1.00 | 63.13 |
| ATOM | 5155 | O | HOH | W | 238 | 20.474  | 17.609 | 84.838 | 1.00 | 57.33 |
| ATOM | 5156 | O | HOH | W | 239 | 25.472  | 69.148 | 91.574 | 1.00 | 49.69 |
| ATOM | 5157 | O | HOH | W | 240 | 26.931  | 38.921 | 43.687 | 1.00 | 43.43 |
| ATOM | 5158 | O | HOH | W | 241 | 41.146  | 39.236 | 69.351 | 1.00 | 51.35 |
| ATOM | 5159 | O | HOH | W | 242 | -15.188 | 39.591 | 69.499 | 1.00 | 52.14 |
| ATOM | 5160 | O | HOH | W | 243 | 38.020  | 68.348 | 72.041 | 1.00 | 63.17 |
| ATOM | 5161 | O | HOH | W | 244 | 37.090  | 47.070 | 57.295 | 1.00 | 67.21 |
| ATOM | 5162 | O | HOH | W | 245 | 14.523  | 42.814 | 79.612 | 1.00 | 50.83 |
| ATOM | 5163 | O | HOH | W | 246 | 21.479  | 71.752 | 81.603 | 1.00 | 57.85 |
| ATOM | 5164 | O | HOH | W | 247 | 3.569   | 32.515 | 42.599 | 1.00 | 63.63 |
| ATOM | 5165 | O | HOH | W | 248 | 15.427  | 30.206 | 95.160 | 1.00 | 66.30 |
| ATOM | 5166 | O | HOH | W | 249 | 17.547  | 60.509 | 94.759 | 1.00 | 68.80 |
| ATOM | 5167 | O | HOH | W | 250 | -20.576 | 43.652 | 41.549 | 1.00 | 58.89 |
| ATOM | 5168 | O | HOH | W | 251 | 26.697  | 43.654 | 74.283 | 1.00 | 50.83 |
| ATOM | 5169 | O | HOH | W | 252 | 0.000   | 75.309 | 76.429 | 1.00 | 53.17 |
| ATOM | 5170 | O | HOH | W | 253 | -6.860  | 59.055 | 50.820 | 1.00 | 52.72 |
| ATOM | 5171 | O | HOH | W | 254 | 19.908  | 76.292 | 86.992 | 1.00 | 57.00 |
| ATOM | 5172 | O | HOH | W | 255 | 15.432  | 77.576 | 52.312 | 1.00 | 58.58 |
| ATOM | 5173 | O | HOH | W | 256 | -1.312  | 22.878 | 57.690 | 1.00 | 56.89 |
| ATOM | 5174 | O | HOH | W | 257 | 23.302  | 46.362 | 42.752 | 1.00 | 58.41 |
| ATOM | 5175 | O | HOH | W | 258 | -3.935  | 18.515 | 44.302 | 1.00 | 66.77 |
| ATOM | 5176 | O | HOH | W | 259 | -0.906  | 44.854 | 67.260 | 1.00 | 67.33 |
| ATOM | 5177 | O | HOH | W | 260 | 40.522  | 44.781 | 83.968 | 1.00 | 59.16 |
| ATOM | 5178 | O | HOH | W | 261 | 37.813  | 59.910 | 97.629 | 1.00 | 57.01 |
| ATOM | 5179 | O | HOH | W | 262 | 32.677  | 55.701 | 51.474 | 1.00 | 60.55 |
| ATOM | 5180 | O | HOH | W | 263 | -6.595  | 33.217 | 67.706 | 1.00 | 51.41 |
| ATOM | 5181 | O | HOH | W | 264 | -11.801 | 39.738 | 40.656 | 1.00 | 59.31 |
| ATOM | 5182 | O | HOH | W | 265 | 36.812  | 27.197 | 69.252 | 1.00 | 57.45 |
| ATOM | 5183 | O | HOH | W | 266 | 34.193  | 52.692 | 52.115 | 1.00 | 59.13 |
| ATOM | 5184 | O | HOH | W | 267 | 12.588  | 76.023 | 54.027 | 1.00 | 63.98 |
| ATOM | 5185 | O | HOH |   |     |         |        |        |      |       |



|      |      |   |     |   |     |        |        |         |      |       |
|------|------|---|-----|---|-----|--------|--------|---------|------|-------|
| ATOM | 5201 | O | HOH | W | 285 | 2.735  | 42.995 | 80.539  | 1.00 | 57.86 |
| ATOM | 5202 | O | HOH | W | 287 | 19.059 | 69.848 | 56.498  | 1.00 | 56.48 |
| ATOM | 5203 | O | HOH | W | 288 | 36.914 | 56.699 | 72.243  | 1.00 | 58.00 |
| ATOM | 5204 | O | HOH | W | 289 | 35.097 | 38.832 | 50.525  | 1.00 | 54.28 |
| ATOM | 5205 | O | HOH | W | 290 | 33.943 | 40.245 | 49.022  | 1.00 | 68.42 |
| ATOM | 5206 | O | HOH | W | 291 | 6.152  | 36.850 | 91.179  | 1.00 | 29.34 |
| ATOM | 5207 | O | HOH | W | 292 | 1.210  | 46.408 | 69.753  | 1.00 | 38.48 |
| ATOM | 5208 | O | HOH | W | 293 | 36.663 | 66.406 | 83.027  | 1.00 | 33.89 |
| ATOM | 5209 | O | HOH | W | 294 | 25.382 | 33.180 | 85.450  | 1.00 | 30.72 |
| ATOM | 5210 | O | HOH | W | 295 | 48.306 | 49.133 | 87.418  | 1.00 | 40.22 |
| ATOM | 5211 | O | HOH | W | 296 | 14.557 | 46.216 | 72.037  | 1.00 | 30.76 |
| ATOM | 5212 | O | HOH | W | 297 | 44.301 | 51.910 | 93.764  | 1.00 | 39.05 |
| ATOM | 5213 | O | HOH | W | 298 | 18.556 | 45.259 | 82.564  | 1.00 | 36.72 |
| ATOM | 5214 | O | HOH | W | 299 | 9.986  | 28.598 | 45.588  | 1.00 | 39.34 |
| ATOM | 5215 | O | HOH | W | 300 | 13.993 | 19.347 | 83.731  | 1.00 | 37.90 |
| ATOM | 5216 | O | HOH | W | 301 | 9.259  | 17.561 | 61.577  | 1.00 | 41.15 |
| ATOM | 5217 | O | HOH | W | 302 | 16.844 | 18.360 | 52.308  | 1.00 | 46.61 |
| ATOM | 5218 | O | HOH | W | 303 | 38.428 | 39.782 | 90.580  | 1.00 | 44.37 |
| ATOM | 5219 | O | HOH | W | 304 | 32.776 | 39.838 | 87.332  | 1.00 | 44.21 |
| ATOM | 5220 | O | HOH | W | 305 | 22.789 | 57.732 | 68.755  | 1.00 | 51.68 |
| ATOM | 5221 | O | HOH | W | 306 | 44.043 | 48.212 | 96.482  | 1.00 | 37.36 |
| ATOM | 5222 | O | HOH | W | 307 | 21.279 | 43.654 | 74.635  | 1.00 | 49.72 |
| ATOM | 5223 | O | HOH | W | 308 | 38.221 | 36.657 | 87.583  | 1.00 | 38.29 |
| ATOM | 5224 | O | HOH | W | 309 | 21.723 | 73.282 | 87.385  | 1.00 | 34.04 |
| ATOM | 5225 | O | HOH | W | 310 | 8.168  | 76.237 | 56.157  | 1.00 | 39.31 |
| ATOM | 5226 | O | HOH | W | 311 | -2.729 | 38.458 | 40.852  | 1.00 | 41.02 |
| ATOM | 5227 | O | HOH | W | 312 | 20.996 | 69.427 | 84.795  | 1.00 | 45.18 |
| ATOM | 5228 | O | HOH | W | 313 | 35.296 | 17.312 | 67.460  | 1.00 | 38.26 |
| ATOM | 5229 | O | HOH | W | 314 | 24.302 | 29.892 | 85.644  | 1.00 | 49.45 |
| ATOM | 5230 | O | HOH | W | 315 | 4.052  | 59.432 | 64.567  | 1.00 | 34.47 |
| ATOM | 5231 | O | HOH | W | 316 | 14.725 | 36.807 | 89.553  | 1.00 | 33.91 |
| ATOM | 5232 | O | HOH | W | 317 | 7.686  | 31.868 | 42.750  | 1.00 | 40.32 |
| ATOM | 5233 | O | HOH | W | 318 | 39.969 | 51.055 | 103.431 | 1.00 | 41.02 |
| ATOM | 5234 | O | HOH | W | 319 | 18.713 | 58.281 | 59.231  | 1.00 | 43.03 |
| ATOM | 5235 | O | HOH | W | 320 | 21.582 | 25.291 | 53.208  | 1.00 | 44.80 |
| ATOM | 5236 | O | HOH | W | 321 | 17.652 | 14.233 | 77.724  | 1.00 | 45.13 |
| ATOM | 5237 | O | HOH | W | 322 | 22.090 | 36.433 | 86.993  | 1.00 | 42.48 |
| ATOM | 5238 | O | HOH | W | 323 | 26.563 | 15.758 | 79.414  | 1.00 | 56.46 |
| ATOM | 5239 | O | HOH | W | 324 | 21.935 | 20.097 | 82.429  | 1.00 | 35.42 |
| ATOM | 5240 | O | HOH | W | 325 | 25.721 | 69.631 | 83.521  | 1.00 | 42.41 |
| ATOM | 5241 | O | HOH | W | 326 | -5.448 | 20.604 | 56.597  | 1.00 | 38.44 |
| ATOM | 5242 | O | HOH | W | 327 | 15.730 | 48.094 | 46.732  | 1.00 | 48.34 |
| ATOM | 5243 | O | HOH |   |     |        |        |         |      |       |



00422410:003609

|      |      |   |           |         |        |         |      |       |
|------|------|---|-----------|---------|--------|---------|------|-------|
| ATOM | 5259 | O | HOH W 344 | 16.842  | 68.765 | 79.662  | 1.00 | 36.62 |
| ATOM | 5260 | O | HOH W 345 | 31.764  | 31.143 | 83.301  | 1.00 | 39.76 |
| ATOM | 5261 | O | HOH W 346 | -21.720 | 43.895 | 50.038  | 1.00 | 56.98 |
| ATOM | 5262 | O | HOH W 347 | 17.485  | 62.993 | 50.436  | 1.00 | 35.10 |
| ATOM | 5263 | O | HOH W 348 | 39.499  | 40.948 | 88.883  | 1.00 | 33.45 |
| ATOM | 5264 | O | HOH W 349 | 11.734  | 28.705 | 89.825  | 1.00 | 45.56 |
| ATOM | 5265 | O | HOH W 350 | 20.754  | 54.796 | 95.357  | 1.00 | 37.52 |
| ATOM | 5266 | O | HOH W 351 | 4.838   | 65.330 | 69.568  | 1.00 | 33.41 |
| ATOM | 5267 | O | HOH W 352 | 33.883  | 66.237 | 72.688  | 1.00 | 33.83 |
| ATOM | 5268 | O | HOH W 353 | 16.037  | 63.226 | 65.963  | 1.00 | 50.85 |
| ATOM | 5269 | O | HOH W 354 | 1.209   | 32.211 | 69.349  | 1.00 | 45.93 |
| ATOM | 5270 | O | HOH W 355 | 25.516  | 49.158 | 94.608  | 1.00 | 47.62 |
| ATOM | 5271 | O | HOH W 356 | 34.387  | 23.584 | 75.231  | 1.00 | 41.51 |
| ATOM | 5272 | O | HOH W 357 | 15.835  | 59.854 | 57.321  | 1.00 | 32.92 |
| ATOM | 5273 | O | HOH W 358 | 30.989  | 22.782 | 58.631  | 1.00 | 48.50 |
| ATOM | 5274 | O | HOH W 359 | -0.131  | 41.666 | 76.726  | 1.00 | 37.81 |
| ATOM | 5275 | O | HOH W 360 | 30.317  | 39.711 | 83.800  | 1.00 | 58.87 |
| ATOM | 5276 | O | HOH W 361 | 22.930  | 24.158 | 51.286  | 1.00 | 40.78 |
| ATOM | 5277 | O | HOH W 362 | 30.355  | 42.190 | 67.705  | 1.00 | 40.91 |
| ATOM | 5278 | O | HOH W 363 | 22.695  | 46.247 | 90.678  | 1.00 | 33.83 |
| ATOM | 5279 | O | HOH W 364 | -20.095 | 25.789 | 45.499  | 1.00 | 46.00 |
| ATOM | 5280 | O | HOH W 365 | 37.366  | 40.766 | 55.105  | 1.00 | 50.47 |
| ATOM | 5281 | O | HOH W 366 | 31.614  | 19.770 | 76.528  | 1.00 | 46.77 |
| ATOM | 5282 | O | HOH W 367 | 28.619  | 21.148 | 76.426  | 1.00 | 45.17 |
| ATOM | 5283 | O | HOH W 368 | 20.788  | 46.785 | 81.907  | 1.00 | 40.07 |
| ATOM | 5284 | O | HOH W 369 | 19.067  | 59.674 | 60.682  | 1.00 | 52.39 |
| ATOM | 5285 | O | HOH W 370 | 17.251  | 57.498 | 44.041  | 1.00 | 42.11 |
| ATOM | 5286 | O | HOH W 371 | 22.814  | 55.956 | 95.276  | 1.00 | 38.36 |
| ATOM | 5287 | O | HOH W 372 | 11.797  | 60.063 | 42.321  | 1.00 | 41.37 |
| ATOM | 5288 | O | HOH W 373 | 4.192   | 63.375 | 62.773  | 1.00 | 41.59 |
| ATOM | 5289 | O | HOH W 374 | -15.434 | 22.581 | 44.545  | 1.00 | 61.31 |
| ATOM | 5290 | O | HOH W 375 | 39.636  | 37.500 | 68.055  | 1.00 | 34.01 |
| ATOM | 5291 | O | HOH W 376 | 22.288  | 40.161 | 68.751  | 1.00 | 47.41 |
| ATOM | 5292 | O | HOH W 377 | -14.370 | 39.668 | 66.900  | 1.00 | 45.13 |
| ATOM | 5293 | O | HOH W 378 | 29.957  | 64.249 | 94.360  | 1.00 | 53.97 |
| ATOM | 5294 | O | HOH W 379 | 16.644  | 14.303 | 57.098  | 1.00 | 53.71 |
| ATOM | 5295 | O | HOH W 380 | 28.540  | 69.064 | 76.673  | 1.00 | 48.14 |
| ATOM | 5296 | O | HOH W 381 | 5.575   | 48.072 | 80.755  | 1.00 | 41.30 |
| ATOM | 5297 | O | HOH W 382 | -3.209  | 37.330 | 44.030  | 1.00 | 38.14 |
| ATOM | 5298 | O | HOH W 383 | 10.772  | 71.014 | 58.445  | 1.00 | 52.05 |
| ATOM | 5299 | O | HOH W 384 | 20.473  | 46.333 | 77.273  | 1.00 | 44.37 |
| ATOM | 5300 | O | HOH W 385 | 25.473  | 45.291 | 93.863  | 1.00 | 39.80 |
| ATOM | 5301 | O | HOH W 386 | 16.812  | 61.299 | 59.570  | 1.00 | 34.64 |
| ATOM | 5302 | O | HOH W 387 | 37.014  | 51.364 | 61.433  | 1.00 | 56.70 |
| ATOM | 5303 | O | HOH W 388 | 12.204  | 59.709 | 63.330  | 1.00 | 41.06 |
| ATOM | 5304 | O | HOH W 389 | 24.023  | 66.534 | 52.905  | 1.00 | 55.32 |
| ATOM | 5305 | O | HOH W 390 | 0.506   | 54.311 | 70.323  | 1.00 | 38.98 |
| ATOM | 5306 | O | HOH W 391 | 11.949  | 16.758 | 53.986  | 1.00 | 53.18 |
| ATOM | 5307 | O | HOH W 392 | 37.416  | 54.792 | 101.784 | 1.00 | 38.65 |
| ATOM | 5308 | O | HOH W 393 | 46.378  | 52.835 | 83.600  | 1.00 | 50.43 |
| ATOM | 5309 | O | HOH W 394 | 24.103  | 26.795 | 86.273  | 1.00 | 49.03 |
| ATOM | 5310 | O | HOH W 395 | 27.075  | 52.383 | 96.106  | 1.00 | 57.28 |
| ATOM | 5311 | O | HOH W 396 | 36.006  | 34.016 | 54.586  | 1.00 | 44.84 |
| ATOM | 5312 | O | HOH W 397 | 38.523  | 29.031 | 71.925  | 1.00 | 33.93 |
| ATOM | 5313 | O | HOH W 398 | 12.523  | 44.136 | 75.273  | 1.00 | 53.61 |
| ATOM | 5314 | O | HOH W 399 | 15.735  | 61.114 | 45.742  | 1.00 | 44.69 |
| ATOM | 5315 | O | HOH W 400 | 20.754  | 35.092 | 42.445  | 1.00 | 51.37 |
| ATOM | 5316 | O | HOH W 401 | 14.222  | 23.180 | 85.491  | 1.00 | 35.20 |



|      |      |   |     |   |     |         |        |         |      |       |
|------|------|---|-----|---|-----|---------|--------|---------|------|-------|
| ATOM | 5317 | O | HOH | W | 402 | -20.951 | 42.853 | 52.762  | 1.00 | 39.02 |
| ATOM | 5318 | O | HOH | W | 403 | 6.053   | 28.199 | 51.239  | 1.00 | 65.04 |
| ATOM | 5319 | O | HOH | W | 404 | 35.313  | 44.557 | 54.005  | 1.00 | 50.04 |
| ATOM | 5320 | O | HOH | W | 405 | -18.153 | 20.676 | 43.582  | 1.00 | 43.52 |
| ATOM | 5321 | O | HOH | W | 406 | 28.895  | 14.049 | 64.120  | 1.00 | 43.99 |
| ATOM | 5322 | O | HOH | W | 407 | 21.077  | 65.132 | 59.088  | 1.00 | 45.25 |
| ATOM | 5323 | O | HOH | W | 408 | 25.918  | 65.162 | 56.853  | 1.00 | 55.28 |
| ATOM | 5324 | O | HOH | W | 409 | 2.421   | 65.212 | 63.670  | 1.00 | 61.93 |
| ATOM | 5325 | O | HOH | W | 410 | -0.547  | 35.743 | 54.699  | 1.00 | 46.69 |
| ATOM | 5326 | O | HOH | W | 411 | -22.289 | 27.518 | 46.814  | 1.00 | 47.50 |
| ATOM | 5327 | O | HOH | W | 412 | 24.607  | 7.260  | 70.646  | 1.00 | 36.92 |
| ATOM | 5328 | O | HOH | W | 413 | 34.593  | 44.376 | 64.986  | 1.00 | 49.97 |
| ATOM | 5329 | O | HOH | W | 414 | 34.413  | 34.797 | 52.195  | 1.00 | 48.85 |
| ATOM | 5330 | O | HOH | W | 415 | -4.740  | 52.565 | 44.026  | 1.00 | 44.22 |
| ATOM | 5331 | O | HOH | W | 416 | 19.232  | 52.944 | 93.963  | 1.00 | 39.51 |
| ATOM | 5332 | O | HOH | W | 417 | 27.621  | 46.196 | 69.991  | 1.00 | 42.91 |
| ATOM | 5333 | O | HOH | W | 418 | 3.480   | 62.682 | 56.725  | 1.00 | 40.03 |
| ATOM | 5334 | O | HOH | W | 419 | 1.599   | 67.083 | 71.072  | 1.00 | 36.73 |
| ATOM | 5335 | O | HOH | W | 420 | 24.962  | 34.424 | 45.256  | 1.00 | 53.29 |
| ATOM | 5336 | O | HOH | W | 421 | 16.185  | 47.345 | 82.105  | 1.00 | 47.82 |
| ATOM | 5337 | O | HOH | W | 422 | 16.038  | 41.047 | 91.569  | 1.00 | 65.77 |
| ATOM | 5338 | O | HOH | W | 423 | 29.831  | 56.603 | 59.633  | 1.00 | 57.12 |
| ATOM | 5339 | O | HOH | W | 424 | 23.000  | 40.491 | 73.243  | 1.00 | 46.62 |
| ATOM | 5340 | O | HOH | W | 425 | 36.125  | 35.327 | 85.790  | 1.00 | 44.47 |
| ATOM | 5341 | O | HOH | W | 426 | 3.089   | 58.590 | 85.674  | 1.00 | 48.29 |
| ATOM | 5342 | O | HOH | W | 427 | -0.907  | 70.074 | 48.963  | 1.00 | 43.00 |
| ATOM | 5343 | O | HOH | W | 428 | -11.044 | 52.085 | 60.685  | 1.00 | 56.36 |
| ATOM | 5344 | O | HOH | W | 429 | 23.496  | 7.025  | 68.752  | 1.00 | 43.76 |
| ATOM | 5345 | O | HOH | W | 430 | -5.598  | 43.223 | 41.100  | 1.00 | 45.62 |
| ATOM | 5346 | O | HOH | W | 431 | 20.167  | 50.377 | 89.978  | 1.00 | 59.50 |
| ATOM | 5347 | O | HOH | W | 432 | -20.425 | 23.096 | 45.440  | 1.00 | 44.34 |
| ATOM | 5348 | O | HOH | W | 433 | 9.260   | 76.289 | 58.173  | 1.00 | 45.95 |
| ATOM | 5349 | O | HOH | W | 434 | -11.917 | 29.670 | 59.131  | 1.00 | 43.37 |
| ATOM | 5350 | O | HOH | W | 435 | 33.178  | 32.939 | 82.506  | 1.00 | 45.21 |
| ATOM | 5351 | O | HOH | W | 436 | 12.256  | 17.158 | 87.387  | 1.00 | 52.47 |
| ATOM | 5352 | O | HOH | W | 437 | 13.785  | 47.874 | 75.233  | 1.00 | 42.67 |
| ATOM | 5353 | O | HOH | W | 438 | 23.499  | 28.449 | 84.993  | 1.00 | 49.95 |
| ATOM | 5354 | O | HOH | W | 439 | 32.378  | 58.281 | 58.965  | 1.00 | 38.63 |
| ATOM | 5355 | O | HOH | W | 440 | 16.415  | 52.385 | 87.735  | 1.00 | 45.19 |
| ATOM | 5356 | O | HOH | W | 441 | -4.177  | 56.799 | 49.770  | 1.00 | 38.37 |
| ATOM | 5357 | O | HOH | W | 442 | 43.834  | 51.522 | 97.318  | 1.00 | 15.87 |
| ATOM | 5358 | O | HOH | W | 443 | 40.609  | 50.537 | 98.000  | 1.00 | 13.87 |
| ATOM | 5359 | O | HOH | W | 444 | 26.131  | 32.974 | 75.528  | 1.00 | 17.75 |
| ATOM | 5360 | O | HOH | W | 445 | 7.172   | 22.314 | 69.284  | 1.00 | 19.18 |
| ATOM | 5361 | O | HOH | W | 446 | 36.875  | 66.145 | 79.032  | 1.00 | 15.68 |
| ATOM | 5362 | O | HOH | W | 447 | 12.570  | 36.470 | 59.739  | 1.00 | 22.25 |
| ATOM | 5363 | O | HOH | W | 448 | 3.629   | 36.729 | 59.008  | 1.00 | 24.63 |
| ATOM | 5364 | O | HOH | W | 449 | 13.223  | 30.168 | 61.997  | 1.00 | 21.63 |
| ATOM | 5365 | O | HOH | W | 450 | 42.538  | 52.950 | 90.812  | 1.00 | 21.87 |
| ATOM | 5366 | O | HOH | W | 451 | 40.673  | 52.006 | 101.288 | 1.00 | 21.07 |
| ATOM | 5367 | O | HOH | W | 452 | 15.152  | 48.019 | 69.852  | 1.00 | 20.74 |
| ATOM | 5368 | O | HOH | W | 453 | 11.735  | 62.018 | 52.859  | 1.00 | 25.04 |
| ATOM | 5369 | O | HOH | W | 454 | 17.367  | 41.418 | 54.225  | 1.00 | 26.89 |
| ATOM | 5370 | O | HOH | W | 455 | 28.048  | 31.054 | 67.049  | 1.00 | 20.41 |
| ATOM | 5371 | O | HOH | W | 456 | 2.679   | 41.086 | 60.234  | 1.00 | 22.58 |
| ATOM | 5372 | O | HOH | W | 457 | 5.044   | 48.874 | 63.550  | 1.00 | 24.48 |
| ATOM | 5373 | O | HOH | W | 458 | 19.970  | 48.260 | 84.436  | 1.00 | 19.72 |
| ATOM | 5374 | O | HOH | W | 459 | 24.119  | 64.991 | 90.851  | 1.00 | 27.81 |



66360-016603

|      |      |   |           |        |        |         |      |       |
|------|------|---|-----------|--------|--------|---------|------|-------|
| ATOM | 5375 | O | HOH W 460 | 27.735 | 64.900 | 76.010  | 1.00 | 22.50 |
| ATOM | 5376 | O | HOH W 461 | 35.183 | 67.097 | 77.274  | 1.00 | 20.47 |
| ATOM | 5377 | O | HOH W 462 | 40.016 | 67.442 | 82.803  | 1.00 | 30.25 |
| ATOM | 5378 | O | HOH W 463 | 21.431 | 20.406 | 79.512  | 1.00 | 19.80 |
| ATOM | 5379 | O | HOH W 464 | 9.801  | 21.726 | 85.048  | 1.00 | 31.87 |
| ATOM | 5380 | O | HOH W 465 | 12.099 | 51.319 | 43.678  | 1.00 | 32.13 |
| ATOM | 5381 | O | HOH W 466 | 21.479 | 47.570 | 79.573  | 1.00 | 20.70 |
| ATOM | 5382 | O | HOH W 467 | 30.644 | 44.679 | 73.638  | 1.00 | 31.20 |
| ATOM | 5383 | O | HOH W 468 | 12.649 | 37.474 | 63.305  | 1.00 | 20.96 |
| ATOM | 5384 | O | HOH W 469 | 17.679 | 67.340 | 77.339  | 1.00 | 31.69 |
| ATOM | 5385 | O | HOH W 470 | 42.001 | 40.231 | 84.180  | 1.00 | 25.43 |
| ATOM | 5386 | O | HOH W 471 | 5.346  | 25.312 | 56.052  | 1.00 | 27.05 |
| ATOM | 5387 | O | HOH W 472 | 24.008 | 46.111 | 79.563  | 1.00 | 24.38 |
| ATOM | 5388 | O | HOH W 473 | 11.126 | 59.092 | 68.572  | 1.00 | 33.24 |
| ATOM | 5389 | O | HOH W 474 | 10.233 | 25.426 | 87.360  | 1.00 | 27.17 |
| ATOM | 5390 | O | HOH W 475 | 10.149 | 53.345 | 78.704  | 1.00 | 29.56 |
| ATOM | 5391 | O | HOH W 476 | 1.207  | 43.652 | 68.278  | 1.00 | 26.00 |
| ATOM | 5392 | O | HOH W 477 | 12.018 | 17.344 | 61.729  | 1.00 | 27.50 |
| ATOM | 5393 | O | HOH W 478 | 39.964 | 44.018 | 89.513  | 1.00 | 25.69 |
| ATOM | 5394 | O | HOH W 479 | 31.106 | 68.340 | 81.212  | 1.00 | 20.95 |
| ATOM | 5395 | O | HOH W 480 | 9.540  | 56.742 | 68.398  | 1.00 | 22.40 |
| ATOM | 5396 | O | HOH W 481 | 40.376 | 40.423 | 86.930  | 1.00 | 24.01 |
| ATOM | 5397 | O | HOH W 482 | 10.453 | 46.869 | 72.971  | 1.00 | 28.43 |
| ATOM | 5398 | O | HOH W 483 | 35.835 | 66.005 | 74.702  | 1.00 | 22.47 |
| ATOM | 5399 | O | HOH W 484 | 16.339 | 37.719 | 53.138  | 1.00 | 23.36 |
| ATOM | 5400 | O | HOH W 485 | 11.797 | 65.996 | 87.056  | 1.00 | 30.00 |
| ATOM | 5401 | O | HOH W 486 | 39.524 | 48.351 | 97.744  | 1.00 | 22.26 |
| ATOM | 5402 | O | HOH W 487 | 34.942 | 31.976 | 64.492  | 1.00 | 32.27 |
| ATOM | 5403 | O | HOH W 488 | 1.032  | 27.223 | 55.074  | 1.00 | 23.57 |
| ATOM | 5404 | O | HOH W 489 | 10.893 | 73.559 | 54.865  | 1.00 | 28.01 |
| ATOM | 5405 | O | HOH W 490 | 16.301 | 57.229 | 55.525  | 1.00 | 30.08 |
| ATOM | 5406 | O | HOH W 491 | 2.296  | 64.458 | 72.194  | 1.00 | 27.27 |
| ATOM | 5407 | O | HOH W 492 | 11.932 | 33.117 | 74.427  | 1.00 | 33.09 |
| ATOM | 5408 | O | HOH W 493 | 26.709 | 61.818 | 82.089  | 1.00 | 25.83 |
| ATOM | 5409 | O | HOH W 494 | 17.635 | 31.832 | 86.739  | 1.00 | 29.42 |
| ATOM | 5410 | O | HOH W 495 | 30.861 | 47.483 | 57.592  | 1.00 | 23.10 |
| ATOM | 5411 | O | HOH W 496 | 19.512 | 53.157 | 91.052  | 1.00 | 24.70 |
| ATOM | 5412 | O | HOH W 497 | 8.653  | 71.188 | 54.342  | 1.00 | 37.16 |
| ATOM | 5413 | O | HOH W 498 | 13.491 | 29.805 | 87.885  | 1.00 | 32.42 |
| ATOM | 5414 | O | HOH W 499 | 28.201 | 17.967 | 60.952  | 1.00 | 27.80 |
| ATOM | 5415 | O | HOH W 500 | 13.916 | 53.020 | 42.749  | 1.00 | 34.25 |
| ATOM | 5416 | O | HOH W 501 | 31.166 | 39.390 | 79.679  | 1.00 | 24.82 |
| ATOM | 5417 | O | HOH W 502 | 17.925 | 47.317 | 76.333  | 1.00 | 23.97 |
| ATOM | 5418 | O | HOH W 503 | 26.920 | 43.271 | 47.865  | 1.00 | 29.84 |
| ATOM | 5419 | O | HOH W 504 | 19.244 | 18.770 | 54.825  | 1.00 | 29.50 |
| ATOM | 5420 | O | HOH W 505 | 7.488  | 22.912 | 71.742  | 1.00 | 29.50 |
| ATOM | 5421 | O | HOH W 506 | 29.694 | 24.129 | 79.931  | 1.00 | 26.39 |
| ATOM | 5422 | O | HOH W 507 | 16.580 | 53.935 | 65.413  | 1.00 | 23.97 |
| ATOM | 5423 | O | HOH W 508 | 47.802 | 53.813 | 102.291 | 1.00 | 22.45 |
| ATOM | 5424 | O | HOH W 509 | 13.313 | 59.974 | 67.561  | 1.00 | 28.60 |
| ATOM | 5425 | O | HOH W 510 | 31.231 | 48.847 | 69.951  | 1.00 | 40.26 |
| ATOM | 5426 | O | HOH W 511 | 25.597 | 46.283 | 68.073  | 1.00 | 31.31 |
| ATOM | 5427 | O | HOH W 512 | 24.049 | 44.380 | 68.623  | 1.00 | 31.48 |
| ATOM | 5428 | O | HOH W 513 | 42.296 | 47.182 | 85.395  | 1.00 | 32.90 |
| ATOM | 5429 | O | HOH W 514 | 0.663  | 35.872 | 64.023  | 1.00 | 24.98 |
| ATOM | 5430 | O | HOH W 515 | 15.871 | 27.279 | 83.599  | 1.00 | 28.22 |
| ATOM | 5431 | O | HOH W 516 | 32.458 | 35.704 | 83.058  | 1.00 | 36.96 |
| ATOM | 5432 | O | HOH W 517 | 10.338 | 31.191 | 71.389  | 1.00 | 28.72 |



|      |      |   |     |   |     |         |        |        |      |       |
|------|------|---|-----|---|-----|---------|--------|--------|------|-------|
| ATOM | 5433 | O | HOH | W | 518 | 16.441  | 43.991 | 73.068 | 1.00 | 33.48 |
| ATOM | 5434 | O | HOH | W | 519 | 21.382  | 44.079 | 85.715 | 1.00 | 36.47 |
| ATOM | 5435 | O | HOH | W | 520 | -12.204 | 45.119 | 45.339 | 1.00 | 38.99 |
| ATOM | 5436 | O | HOH | W | 521 | 41.850  | 50.387 | 91.395 | 1.00 | 25.85 |
| ATOM | 5437 | O | HOH | W | 522 | 38.157  | 43.711 | 71.143 | 1.00 | 33.79 |
| ATOM | 5438 | O | HOH | W | 523 | 10.857  | 37.770 | 74.674 | 1.00 | 36.91 |
| ATOM | 5439 | O | HOH | W | 524 | 2.452   | 57.926 | 62.203 | 1.00 | 29.86 |
| ATOM | 5440 | O | HOH | W | 525 | 31.918  | 38.240 | 82.071 | 1.00 | 26.60 |
| ATOM | 5441 | O | HOH | W | 526 | 19.394  | 32.573 | 51.517 | 1.00 | 32.52 |
| ATOM | 5442 | O | HOH | W | 527 | 10.970  | 64.850 | 89.305 | 1.00 | 26.44 |
| ATOM | 5443 | O | HOH | W | 528 | 15.768  | 58.372 | 93.236 | 1.00 | 29.74 |
| ATOM | 5444 | O | HOH | W | 529 | 9.811   | 24.439 | 85.111 | 1.00 | 32.52 |
| ATOM | 5445 | O | HOH | W | 530 | 32.677  | 43.807 | 51.972 | 1.00 | 41.47 |
| ATOM | 5446 | O | HOH | W | 531 | 3.498   | 33.335 | 78.392 | 1.00 | 38.95 |
| ATOM | 5447 | O | HOH | W | 532 | 22.765  | 37.334 | 45.311 | 1.00 | 34.30 |
| ATOM | 5448 | O | HOH | W | 533 | 22.289  | 62.694 | 93.625 | 1.00 | 28.38 |
| ATOM | 5449 | O | HOH | W | 534 | 18.456  | 59.233 | 56.401 | 1.00 | 32.51 |
| ATOM | 5450 | O | HOH | W | 535 | 6.870   | 45.103 | 78.168 | 1.00 | 43.85 |
| ATOM | 5451 | O | HOH | W | 536 | 26.869  | 66.922 | 80.584 | 1.00 | 33.36 |
| ATOM | 5452 | O | HOH | W | 537 | 28.274  | 69.424 | 80.635 | 1.00 | 32.22 |
| ATOM | 5453 | O | HOH | W | 538 | 16.644  | 24.985 | 84.601 | 1.00 | 42.11 |
| ATOM | 5454 | O | HOH | W | 539 | 13.875  | 66.937 | 52.609 | 1.00 | 39.81 |
| ATOM | 5455 | O | HOH | W | 540 | 35.698  | 18.768 | 63.774 | 1.00 | 39.08 |
| ATOM | 5456 | O | HOH | W | 541 | 9.604   | 60.060 | 65.965 | 1.00 | 39.46 |
| ATOM | 5457 | O | HOH | W | 542 | -19.968 | 45.560 | 49.328 | 1.00 | 49.42 |
| ATOM | 5458 | O | HOH | W | 543 | 28.747  | 37.637 | 80.667 | 1.00 | 29.83 |
| ATOM | 5459 | O | HOH | W | 544 | 38.122  | 41.611 | 59.189 | 1.00 | 42.35 |
| ATOM | 5460 | O | HOH | W | 545 | 36.168  | 59.639 | 75.298 | 1.00 | 30.81 |
| ATOM | 5461 | O | HOH | W | 546 | 5.231   | 27.744 | 55.129 | 1.00 | 40.94 |
| ATOM | 5462 | O | HOH | W | 547 | 42.358  | 42.723 | 76.149 | 1.00 | 33.83 |
| ATOM | 5463 | O | HOH | W | 548 | 5.149   | 70.452 | 72.761 | 1.00 | 64.99 |
| ATOM | 5464 | O | HOH | W | 549 | 0.638   | 55.495 | 62.775 | 1.00 | 29.98 |
| ATOM | 5465 | O | HOH | W | 550 | 35.051  | 47.144 | 54.258 | 1.00 | 36.91 |
| ATOM | 5466 | O | HOH | W | 551 | 20.979  | 44.359 | 69.352 | 1.00 | 38.48 |
| ATOM | 5467 | O | HOH | W | 552 | 8.699   | 44.016 | 58.770 | 1.00 | 39.13 |
| ATOM | 5468 | O | HOH | W | 553 | 30.041  | 49.977 | 93.866 | 1.00 | 50.89 |
| ATOM | 5469 | O | HOH | W | 554 | 14.340  | 30.254 | 46.134 | 1.00 | 34.10 |
| ATOM | 5470 | O | HOH | W | 555 | 32.981  | 51.053 | 96.313 | 1.00 | 44.00 |
| ATOM | 5471 | O | HOH | W | 556 | 18.695  | 43.789 | 84.698 | 1.00 | 31.02 |
| ATOM | 5472 | O | HOH | W | 557 | 30.439  | 59.776 | 96.480 | 1.00 | 36.06 |
| ATOM | 5473 | O | HOH | W | 558 | 31.888  | 50.518 | 46.532 | 1.00 | 40.30 |
| ATOM | 5474 | O | HOH | W | 559 | 3.242   | 29.430 | 49.193 | 1.00 | 33.03 |
| ATOM | 5475 | O | HOH |   |     |         |        |        |      |       |



|      |      |   |           |        |        |         |      |       |
|------|------|---|-----------|--------|--------|---------|------|-------|
| ATOM | 5491 | O | HOH W 578 | 8.396  | 73.512 | 56.345  | 1.00 | 30.97 |
| ATOM | 5492 | O | HOH W 579 | 3.331  | 27.097 | 72.842  | 1.00 | 45.67 |
| ATOM | 5493 | O | HOH W 580 | 15.169 | 10.135 | 64.570  | 1.00 | 42.16 |
| ATOM | 5494 | O | HOH W 581 | 45.191 | 54.292 | 101.410 | 1.00 | 30.43 |
| ATOM | 5495 | O | HOH W 582 | 26.470 | 57.589 | 66.563  | 1.00 | 39.66 |
| ATOM | 5496 | O | HOH W 583 | 10.893 | 50.001 | 41.681  | 1.00 | 27.20 |
| ATOM | 5497 | O | HOH W 584 | 16.236 | 44.961 | 46.675  | 1.00 | 36.26 |
| ATOM | 5498 | O | HOH W 585 | 30.990 | 43.578 | 71.047  | 1.00 | 45.95 |
| ATOM | 5499 | O | HOH W 586 | 10.763 | 58.258 | 90.908  | 1.00 | 31.78 |
| ATOM | 5500 | O | HOH W 587 | 17.447 | 64.598 | 52.313  | 1.00 | 35.13 |
| ATOM | 5501 | O | HOH W 588 | 40.235 | 53.292 | 74.530  | 1.00 | 51.39 |
| ATOM | 5502 | O | HOH W 589 | 18.908 | 42.622 | 78.518  | 1.00 | 39.32 |
| ATOM | 5503 | O | HOH W 590 | 30.298 | 15.653 | 74.234  | 1.00 | 38.34 |
| ATOM | 5504 | O | HOH W 591 | 31.762 | 51.365 | 51.354  | 1.00 | 47.66 |
| ATOM | 5505 | O | HOH W 593 | 20.876 | 60.082 | 62.179  | 1.00 | 20.00 |
| END  |      |   |           |        |        |         |      |       |

0012210 022509



## CLAIMS

1. An isolated protein comprising at least a subsequence of the amino acid sequence of leukotriene A<sub>4</sub> (LTA<sub>4</sub>) hydrolase and having the corresponding three dimensional form adopted thereof in nature, said subsequence being capable of participating in the control of the an enzymatic pathway, such as the leukotriene cascade, a functionally equivalent part, derivative or conformational analogue thereof.
2. A protein according to claim 1, which is comprised essentially of the amino acid sequence of LTA<sub>4</sub> hydrolase and exhibits the corresponding three-dimensional form adopted thereof in nature, essentially as disclosed in Table 9-11 by the parameters defining atom 1- atom 4876.
3. A protein according to claim 1 or 2, which comprises an enzymatically active site defined in the following table:

|   | Left wall                                 | Right wall                                |
|---|---|---|
| 1 |   | Lys608, Asp606, Lys605,<br>Lys354, Thr355 |
| 2 | Phe356, Phe362                            | Gln544, Asp573, Lys572, Arg568            |
| 3 | Val376                                    | Lys565, Arg540, Leu507                    |
| 4 | Ser380, Ser352, Glu348                    | Pro569                                    |
| 5 | Tyr378, Glu348                            | Arg563, Glu533, Phe536,<br>Arg537, Tyr267 |
| 6 | Tyr383, Phe314, Glu318, Glu384,<br>Arg326 |   |
| 7 | Gly268, Gly269, Met270                    | His295, Asn341, Phe340                    |
| 8 | Ser288, His497                            | Glu325, Asn291                            |

4. A protein according to claim 3, which is an enzyme having a metallohydrolase activity capable of participating in the regulation of enzyme activities in



biochemical pathways, wherein said enzymes have structures similar to the ones defined in claim 3.

5. A protein according to claim 1 or 2, which comprises an enzymatically active site defined by the following amino acids:

Gln136  
Ala137  
Tyr267  
Gly268  
Gly269  
Met270  
Glu271  
Val292  
His295  
Glu296  
His299  
Glu318  
Tyr378  
Tyr383  
Arg563  
Lys565

6. A protein according to claim 1 or 2, which comprises an enzymatically active site defined by the following amino acids:

Gln136  
Ala137  
Tyr267  
Gly268  
Gly269  
Met270  
Glu271  
Val292  
His295  
Glu296  
His299  
Trp315  
Glu318  
Val322  
Phe362  
Val367  
Leu369  
Pro374



Asp375  
Ile372  
Ala377  
Pro382  
Tyr378  
Tyr383  
Arg563  
Lys565

7. A compound which is substantially complementary to a protein according to any one of claims 1-6.
8. A compound according to claim 7, which is substantially complementary to an enzymatically active site of said protein and which is capable of specifically inhibiting said enzymatic activity.
9. A compound according to claim 8, which is an inhibitor of a metallohydrolase enzyme.
10. An isolated complex, which is comprised of a protein according to claim 1-6 and a complementary compound according to any one of claims 7-9, wherein the three-dimensional structure of LTA<sub>4</sub> hydrolase is essentially as disclosed in Tables 9-11 by the parameters defining atom 1- atom 4876, or a functionally equivalent part, derivative or conformational analogue of such a complex.
11. A complex according to claim 10, wherein the protein complexed with LTA<sub>4</sub> hydrolase is the inhibitor bestatin, thiolamine or hydroxamic acid, wherein the three-dimensional structure of said inhibitor is essentially as disclosed in Tables 9-11, or a functionally equivalent part, derivative or conformational analogue of such a complex.
12. Use of a protein according to any one of claims 1-6, a compound according to any one of claims 7-9 or a complex according to claim 10 or 11 in drug design, such as in molecular modeling, direct structure-based design and/or combinatorial chemistry.
13. Use according to claim 12, wherein said drug is for the treatment and/or prevention of disorders involving acute and chronic inflammatory and/or







21. A method for screening LTA<sub>4</sub> hydrolase binding compounds complementary to a region of LTA<sub>4</sub> hydrolase, preferably an enzymatically active site thereof, which comprises the steps of
- (a) producing a multiplicity of possible complementary structures and
  - (b) selecting a structure, wherein the three-dimensional configuration and spatial arrangement of regions involved in binding to LTA<sub>4</sub> hydrolase remain substantially preserved, which selection is based on the three-dimensional structure of LTA<sub>4</sub> hydrolase, and/or LTA<sub>4</sub> hydrolase complexed to an inhibitor thereof, in a form adopted thereof in nature, such as defined in Tables 9-11.
22. A method according to claim 21, wherein a general metallohydrolase inhibitor is selected, which is capable of inhibiting an enzyme belonging to the M1 family.
23. A method according to claim 21, wherein an inhibitor of the epoxide hydrolase activity and/or aminopeptidase activity of LTA<sub>4</sub> hydrolase or of LTC<sub>4</sub> synthases is selected.
24. A method according to claim 21, wherein a compound capable of antagonizing LTB<sub>4</sub> receptor binding of a cell is selected.
25. A compound obtainable by the method according to any one of claims 21-24.
26. A method of engineering a protein, which method comprises the steps of
- identification of a suitable set of mutations based on the structure of LTA<sub>4</sub> hydrolase;
  - generation of a library of genes which contains the suitable sequence variations;
  - selection of clones encoding the LTA<sub>4</sub> hydrolase analogues with a desired activity function;
- wherein said desired activity is the capability of efficiently producing an organic compound of interest.
27. A method according to claim 26, wherein the specified property is the suicidal mode of action of LTA<sub>4</sub> hydrolase.

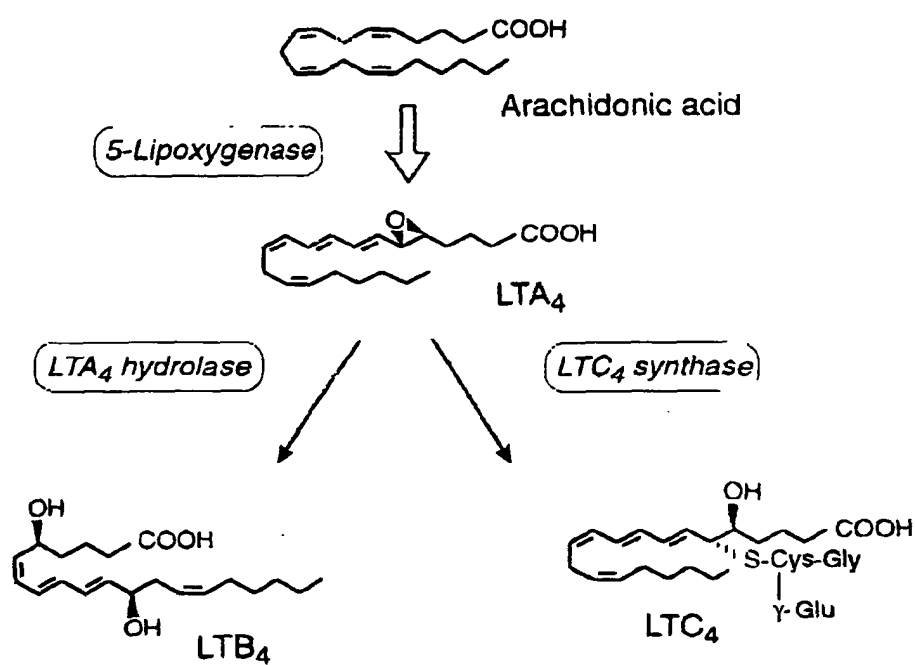


[illegible]

343



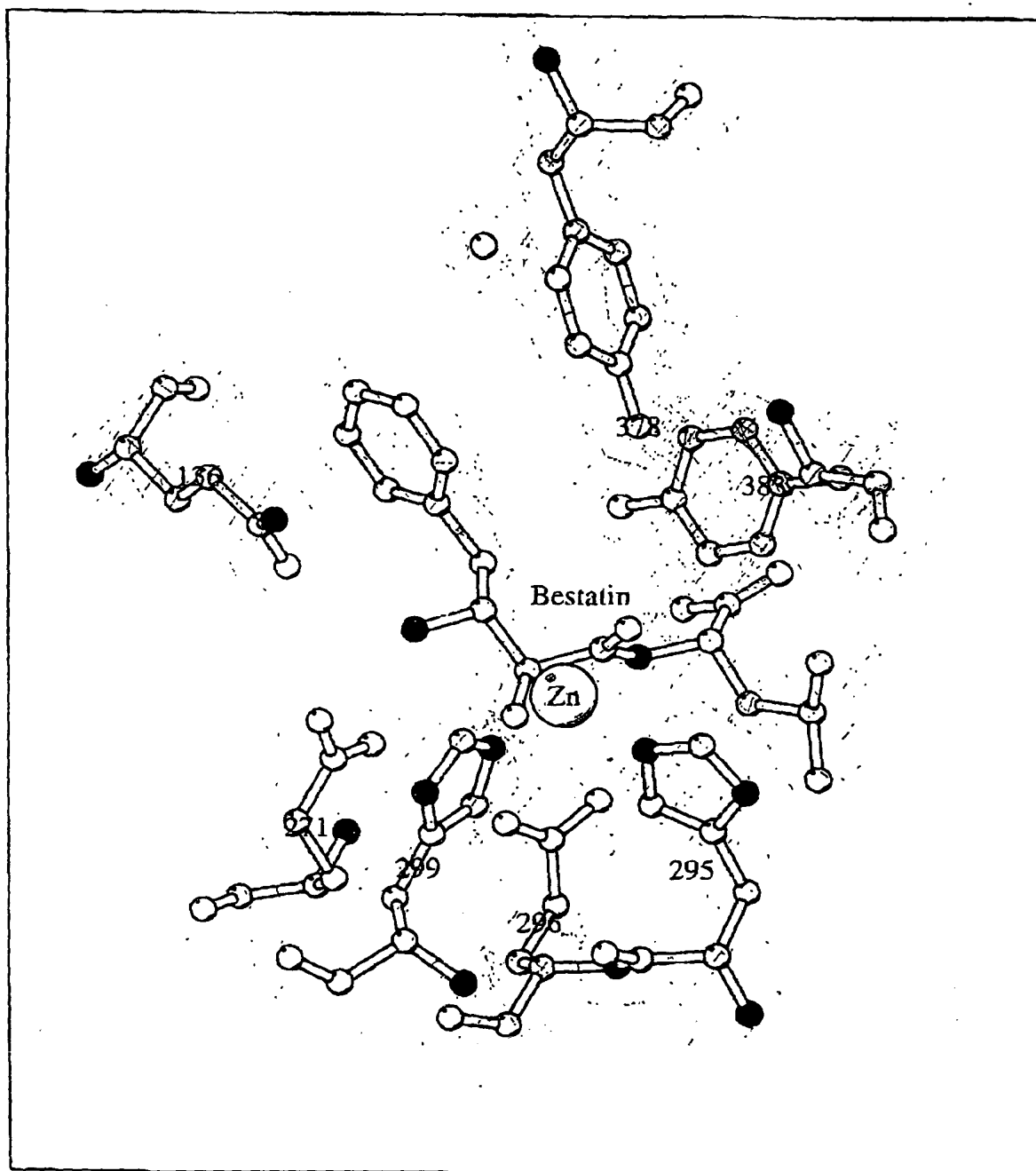
Figure 1





2/14

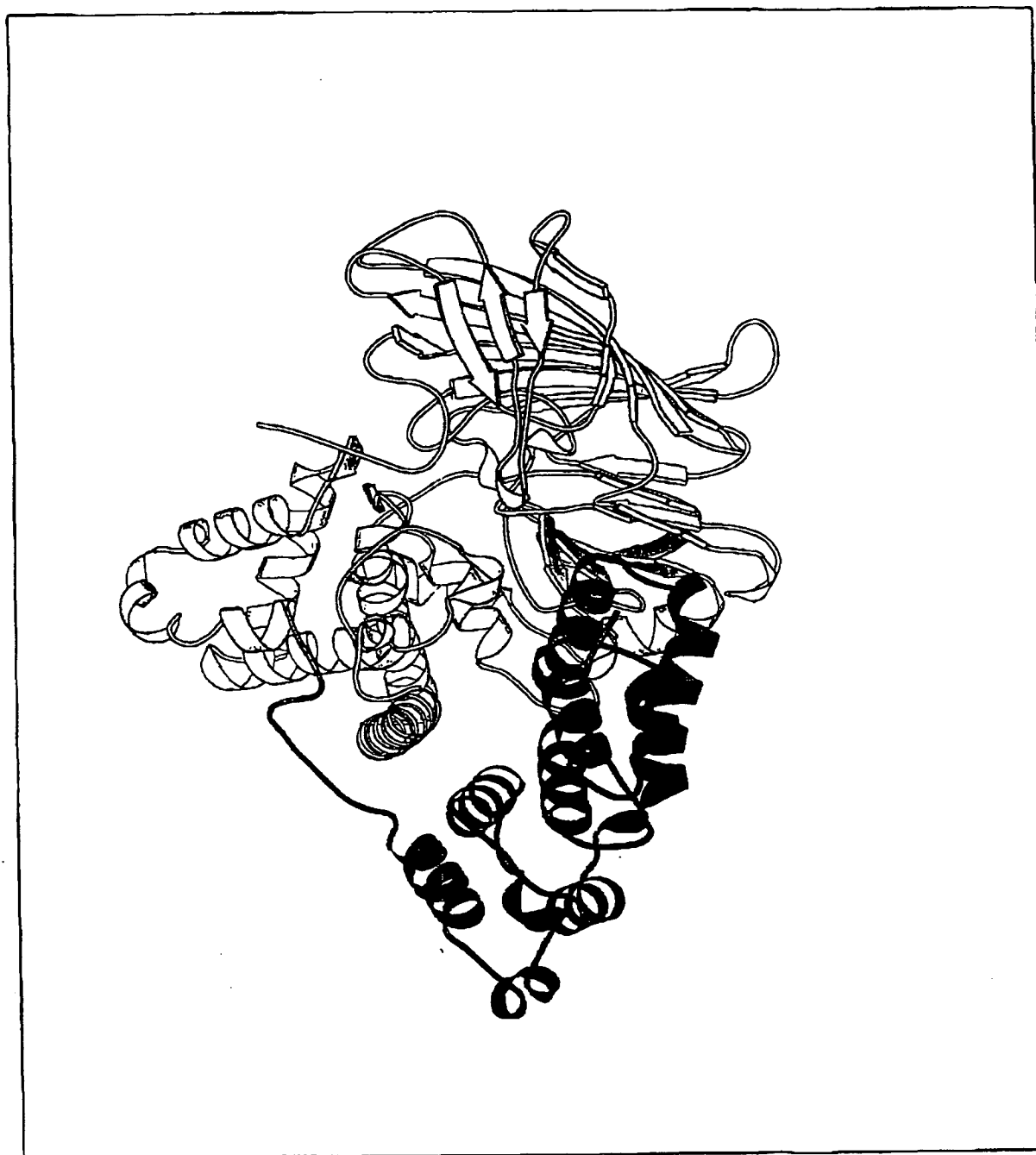
Figure 2





3/14

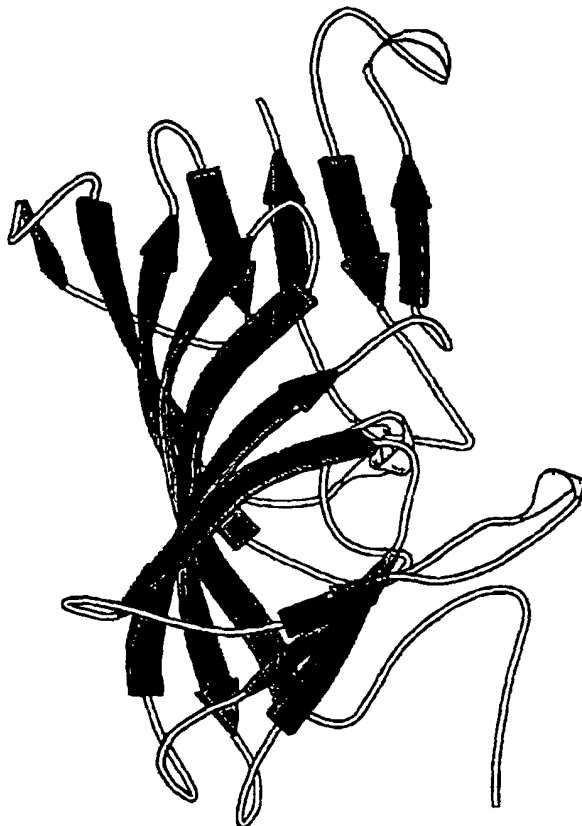
Figure 3



6012310:02600



Figure 4a

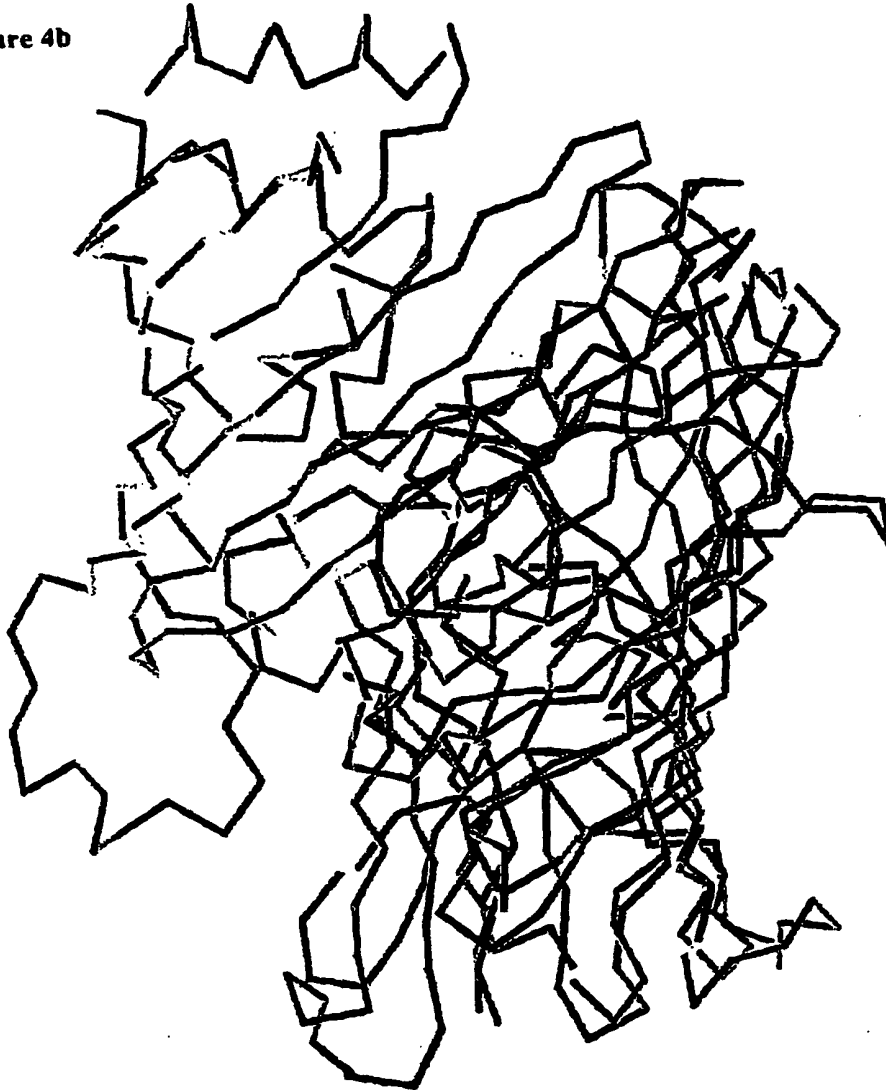


669220-0122109



5/14

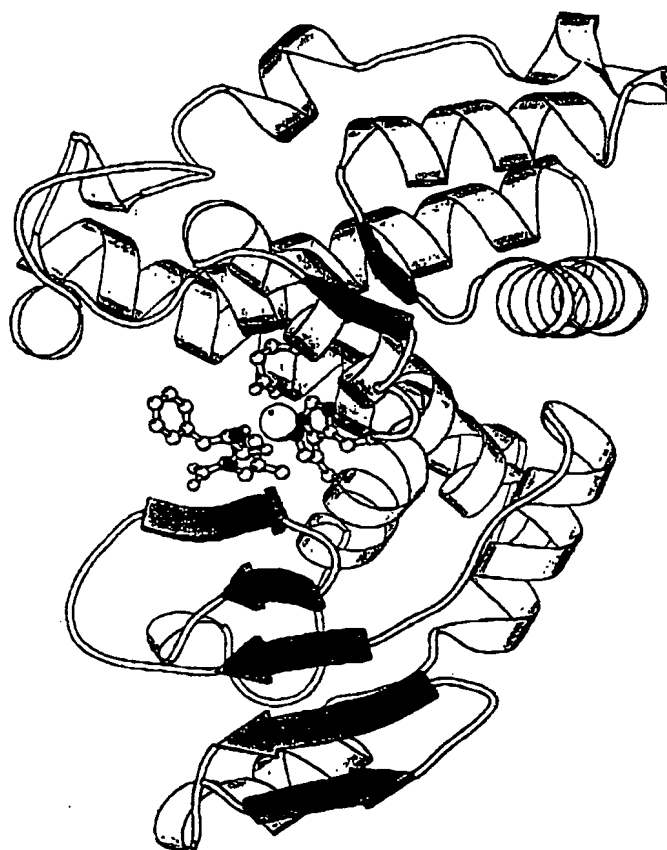
Figure 4b



00000-00000



6/14

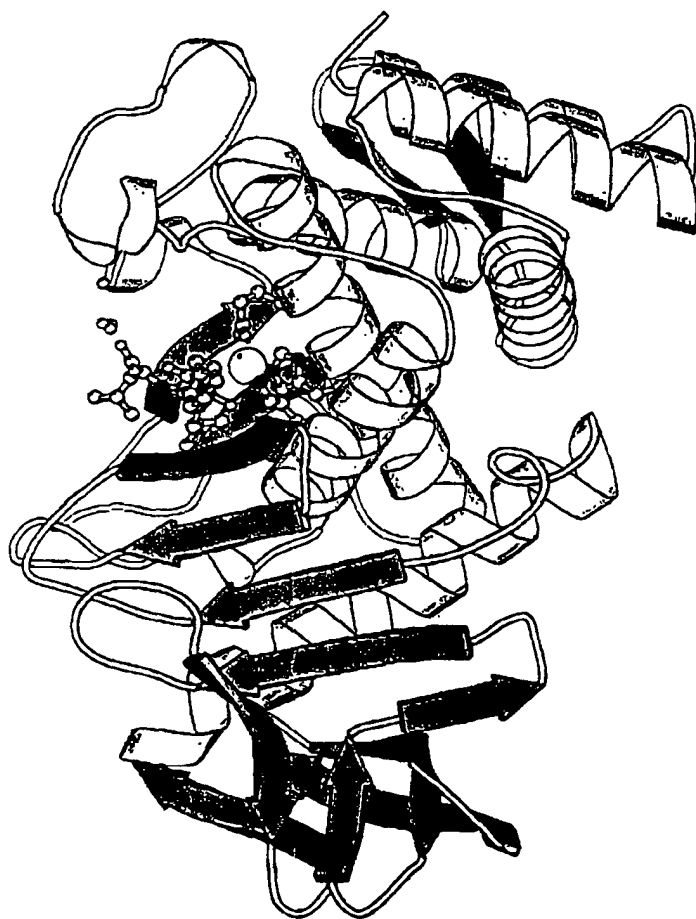
**Figure 5a**

669220 01422109



7/14

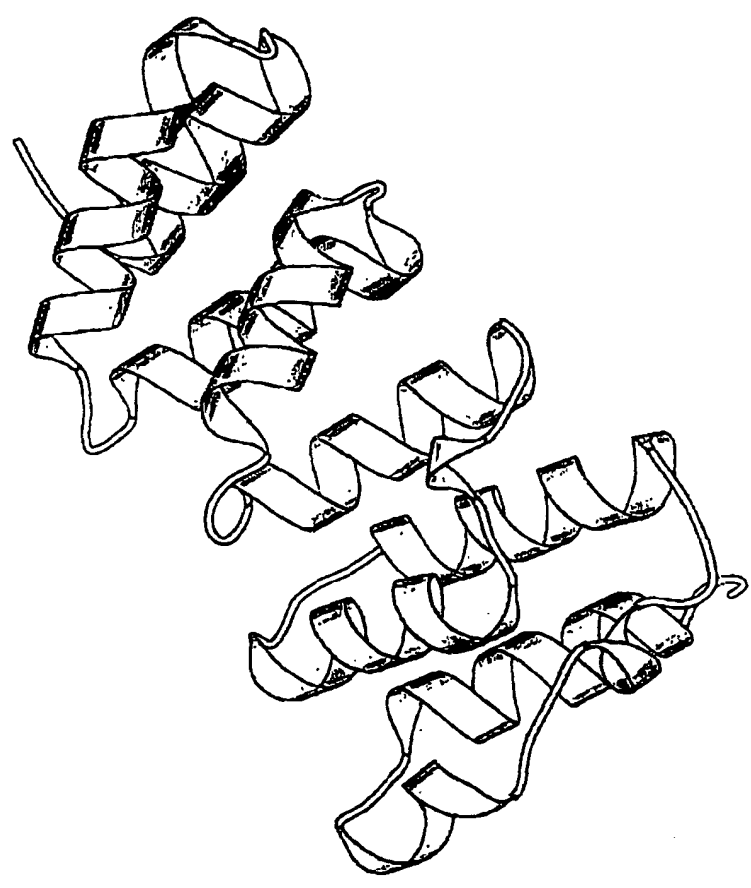
Figure 5b



66322-01-22705



Figure 6

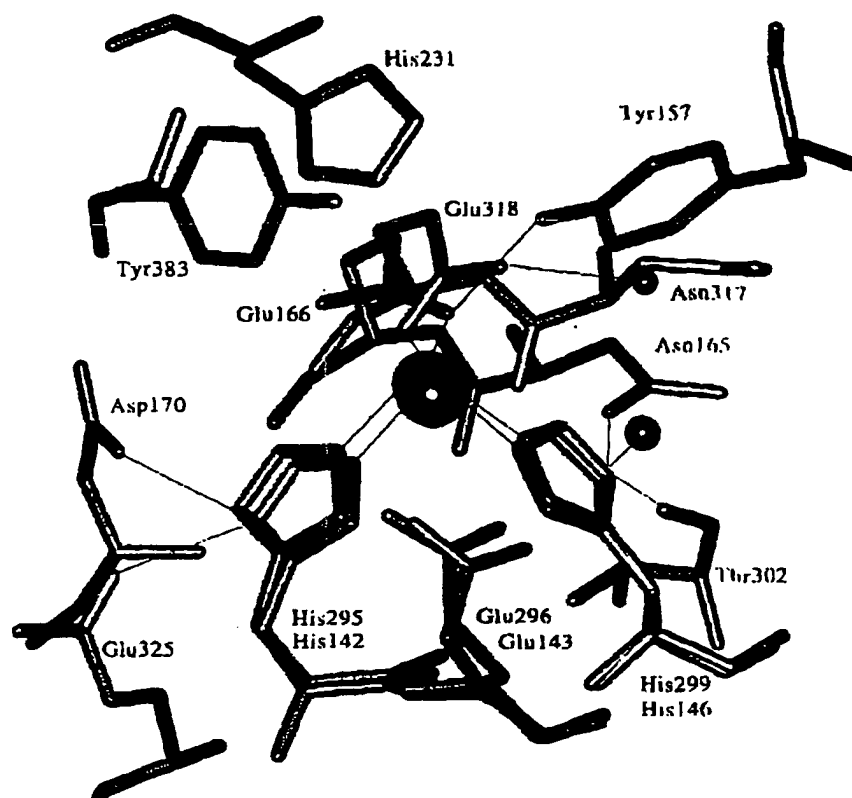


6042410.02369



9/14

Figure 7



601210-02599

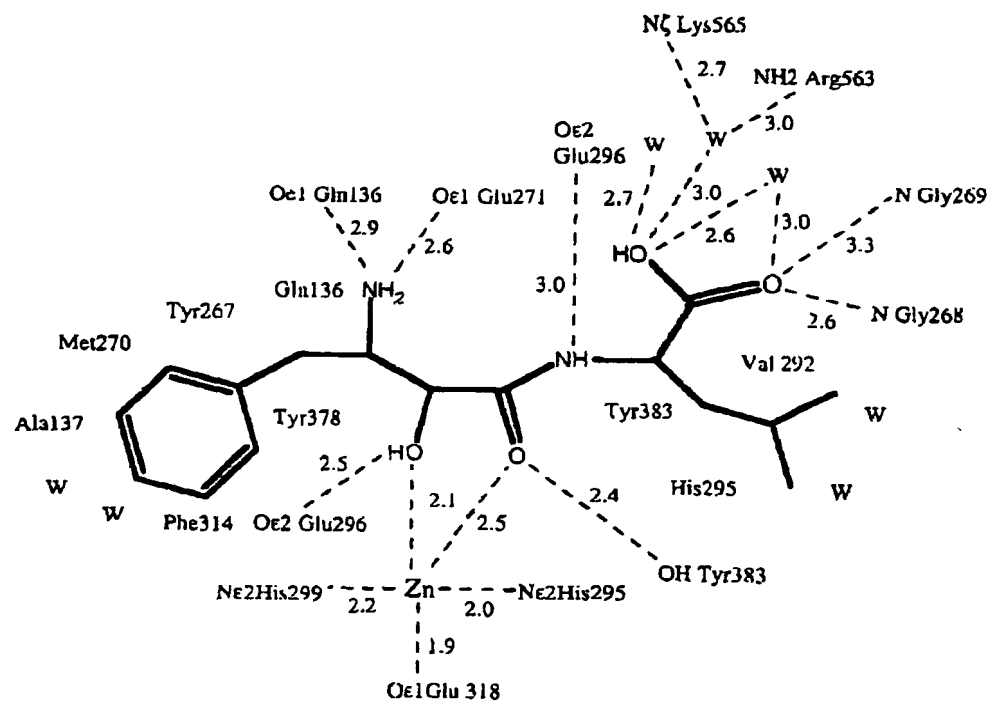






11/14

Figure 8b





12/14

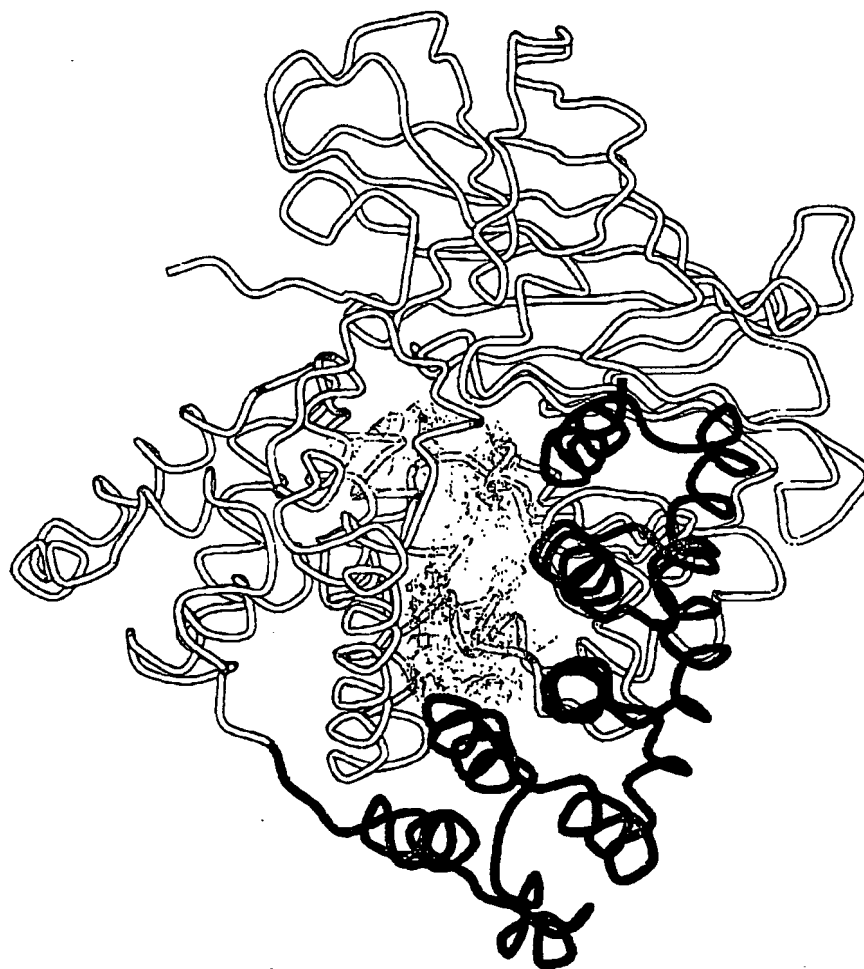
**Figure 9a**



Figure 9b

